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The Water Quality Analysis Simulation Program--3 (WASP3) is a dynamic compartment modeling system that can be used to analyze a variety of water quality problems in a diverse set of water bodies. WASP3 simulates the transport and transformation of conventional and toxic pollutants in the water column and benthos of ponds, lakes, streams, rivers, reservoirs, estuaries, and coastal waters. The WASP3 modeling system covers four major subjects: hydrodynamics, conservative mass transport, eutrophication-dissolved oxygen kinetics, and toxic chemical-sediment dynamics. This manual contains three main parts: Model Theory, User's Manual, and Programmer's Guide. The WASP3 modeling system consists of two stand-alone computer programs, DYNHYD3 and WASP3, that can be run in conjunction or separately. The hydrodynamic program, DYNHYD3, simulates the movement of water and the water quality program simulates the movement and interaction of pollutants within the water. The latter program is supplied with two kinetic submodels to simulate two of the major classes of water quality problems: conventional pollution (dissolved oxygen, biochemical oxygen demand, nutrients, and eutrophication) and toxic pollution (organic chemicals, heavy metals, and sediment). The substitution of either submodel constitutes the models EUTRWASP and TOXIWASP, respectively.

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WASP3, A HYDRODYNAMIC AND WATER QUALITY MODEL--MODEL THEORY, USER'S MANUAL, AND PROGRAMMER'S GUIDE

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient management tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Assessment Branch develops state-of-the-art mathematical models for use in water quality evaluation and management.

The Water Quality Analysis Program (WASP) was developed in 1981 by Dominic Di Toro, James Fitzpatrick, and Robert Thomann of Hydroscience, Inc. (presently Hydroqual, Inc.). Because of its unique flexibility, the model has been widely used throughout the United States to predict water quality responses to natural and man-made pollution. In the work reported here, WASP was updated and combined with a set of eutrophication and toxic chemical subroutines and a hydrodynamics program called DYNHYD3, which is an enhancement of the Potomac Estuary Model developed by Steve Roesch and Leo Clark of EPA Region III's Central Regional Laboratory. The resulting WASP3 modeling system is a powerful tool for simulating the movement of water and the movement and interaction of both conventional and toxic pollutants within the water. Appropriate application of the model will provide valuable information on which to base various pollution management decisions.

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PREFACE

The application of mathematical modeling techniques to water quality problems has proved to be a powerful tool in water resource management. As a diagnostic tool, it permits the abstraction of a highly complex real world. Realizing that no one can ever detail all the physical phenomena that comprise our natural world, the modeler attempts to identify and include only the phenomena, be they natural or man-made, that are relevant to the water quality problem under consideration. As a predictive tool, mathematical modeling permits the forecasting and evaluation of the effects of changes in the surrounding environment on water quality. Although engineering insight and political and socioeconomic concerns play important roles in water resource management, some water quality problems are of such a complex nature that the predictive capability of mathematical models provides the only real means for screening the myriad number of management alternatives.

It is important for a computer program to be very general in nature if it is to serve as the basis for the mathematical modeler. The program should be flexible enough to provide the modeler with the mechanisms to describe and provide input data for the geophysical morphology, the transport processes, and the transformation processes that go into the framework of the model. Transport processes, basically hydrodynamic in nature, include advection, turbulent diffusion, and, when spatial averaging is included, dispersion. Transformation (or reactive) processes, which are the sources and sinks that act upon a particular water quality parameter, may be physical, chemical or biological. Examples of these processes are the sedimentation and flocculation of organics, the assimilative capacity of a water body to receive an acid waste discharge, and the predator-prey relationship of zooplankton-phytoplankton.

The WASP3 modeling system was designed to provide the generality and flexibility necessary for analyzing a variety of water quality problems in a diverse set of water bodies. The particular components described in this manual can be used for the hydrodynamics of large branching rivers, reservoirs, and estuaries; the mass transport in ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters; and the kinetic interactions of eutrophication-dissolved oxygen and sediment-toxic chemicals.

This manual contains three main sections that can be used independently by various members of a modeling team. The first section, WASP3 Model Theory, documents the equations and assumptions underlying the WASP3 model components. Some guidance on the use of these models is offered, along with sample input data values, when appropriate. More general summaries of equations and data are provided in the "Rates Manual" (Bowie et al., 1985) and the "Screening Manual" (Mills et al., 1985). A rates manual for toxic organics and metals is in preparation as of this writing.

The second section, WASP3 User's Manual, documents the input data specifications necessary to run the WASP3 models. Each data group is described, with input variable names, formats, and definitions. Convenient tabular summaries of each data group are provided, followed by an alphabetical listing of variables with short definitions for quick reference.

The third section, WASP3 Programmer's Manual, documents the computer requirements necessary to support the WASP3 models. Hardware and software specifications are given, followed by installation and implementation instructions and a description of command files. A description of the computer programs themselves includes an overview of the system, the computer files, COMMON blocks, subroutines, and overlay structures.

ABSTRACT

The Water Quality Analysis Simulation Program--3 (WASP3) is a dynamic compartment modeling system that can be used to analyze a variety of water quality problems in a diverse set of water bodies. WASP3 simulates the transport and transformation of conventional and toxic pollutants in the water column and benthos of ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters. The WASP3 modeling system covers four major subjects: hydrodynamics, conservative mass transport, eutrophication-dissolved oxygen kinetics, and toxic chemical-sediment dynamics. This manual contains three main parts: Model Theory, User's Manual, and Programmer's Guide.

The WASP3 modeling system consists of two stand-alone computer programs, DYNHYD3 and WASP3, that can be run in conjunction or separately. The hydrodynamic program, DYNHYD3, simulates the movement of water and the water quality program simulates the movement and interaction of pollutants within the water. The latter program is supplied with two kinetic sub-models to simulate two of the major classes of water quality problems: conventional pollution (dissolved oxygen, biochemical oxygen demand, nutrients and eutrophication) and toxic pollution (organic chemicals, heavy metals, and sediment). The substitution of either sub-model constitutes the models EUTRWASP and TOXIWASP, respectively.

This report covers the period October 1, 1984 to June 30, 1986, and work was completed as of June 30, 1986.

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A manual of this type necessarily draws heavily upon the work of others. Part 1--Theory--incorporates much material from four previous manuals on DYNHYD2 (Steve Roesch and Leo Clark), WASP (Dominic DiToro, James Fitzpatrick, and Robert Thomann), the Potomac Eutrophication Model (Robert Thomann and James Fitzpatrick), and TOXIWASP (Robert Ambrose, Sam Hill, and Lee Mulkey). In particular, text for Chapter 1.4 on the eutrophication model is taken with little modification from the PEM documentation report. We gratefully acknowledge Drs. Thomann and Fitzpatrick for this work.

Two technical aides played a large role in organizing and assembling this manual. Joseph Cronk began the task, and Sarah Hussey continued his effort, assembling the original drafts of the User Manual. In addition, Ms. Hussey drafted many of the figures, first for WASP training courses, and then for the manual.

Ms. Annie Smith typed the entire manual in less than two weeks while continuing to serve an entire branch with grace and efficiency. 'Nuff said.

John Connolly has been a popular lecturer in every WASP training course. Some of his course notes have inevitably been incorporated here, particularly in Section 1.3.4 on the basic finite difference implementation.

Finally, we'd like to thank the many users who participated in the courses, shared professional experiences, and offered useful suggestions.

SECTION 1

WASP3 MODEL THEORY

The Water Quality Analysis Simulation Program--3 (WASP3), an enhancement of the original WASP (Di Toro et al., 1983), helps users interpret and predict water quality responses to natural phenomena and man-made pollution for various pollution management decisions. WASP3 is a dynamic compartment modeling program for aquatic systems, including both the water column and the underlying benthos. The time-varying processes of advection, dispersion, point and diffuse mass loading, and boundary exchange are represented in the basic program.

Water quality processes are represented in special kinetic subroutines that are either chosen from a library or written by the user. WASP is structured to permit easy substitution of kinetic subroutines into the overall package to form problem-specific models. Versions of WASP have been used to examine eutrophication and PCB pollution of the Great Lakes (Thomann, 1975; Thomann et al., 1976; Thomann et al., 1979; Di Toro and Connolly, 1980), eutrophication of the Potomac Estuary (Thomann and Fitzpatrick, 1982), kepone pollution of the James River Estuary (O'Connor et al., 1983), volatile organic pollution of the Delaware Estuary (Ambrose, 1986), and heavy metal pollution of the Deep River, North Carolina (JRB, 1984). In addition to these, Table 1 provides a list of applications (Di Toro et al., 1983).

The flexibility afforded by the Water Quality Analysis Simulation Program is unique. WASP3 permits the modeler to structure one, two, and three-dimensional models; allows the specification of time-variable exchange coefficients, advective flows, waste loads and water quality boundary conditions; and permits tailored structuring of the kinetic processes, all within the larger modeling framework without having to write or rewrite large sections of computer code. Although WASP's multidimensionality and time-variable input capabilities are strong points, it is probably the ease with which one may develop new kinetic or reactive structures that is WASP's main strength. WASP's generality, however, requires an additional measure of judgment and insight on the part of the modeler. The kinetic and transport structures are not "hard wired" in WASP (i.e., the equations are not "fixed" and "buried" in the code). Therefore, the burden is on the modeler (perhaps together with a programmer) to write the applicable kinetic equations (or use those already implemented) for a given problem context.

TABLE 1. APPLICATIONS OF WASP PROGRAM

Geographical Area	Spatial Dimensionality	Number of Spatial Segments	Number of State Variables	Principal State Variables	Time Scale	Remarks
Eutrophication Problem Contexts						
Western Delta-Suisun Bay Area of San Francisco Bay	2 Dimensional Laterally	39	11	Chlorophyll, Nigroten, Silica, DO	Week-Week	Original problem setting for development of WASP-1970
Potomac Estuary	2 Dimensional	36	8	Chlorophyll, Nitrogen Phosphorus	Week-Week	
GREAT LAKES						
Lake Ontario	1 Dimensional Vertically	2	13	Chlorophyll, Zooplankton, Phosphorus, Nitrogen, Silica	Week-Week and Year-Year	Lake1 Model
Lake Ontario	3 Dimensional	67	8	Chlorophyll, Zooplankton, Phosphorus, Nitrogen, Silica	Week-Week and Year-Year	Lake3 Model
Rochester Embayment	3 Dimensional	72	8	Chlorophyll, Zooplankton, Phosphorus, Nitrogen, Silica	Week-Week and Year-Year	

TABLE 1. APPLICATIONS OF WASP PROGRAM (Continued)

Geographical Area	Spatial Dimensionality	Number of Spatial Segments	Number of State Variables	Principal State Variables	Time Scale	Remarks
Eutrophication Problem Contexts, Cont.						
Lake Huron	3 Dimensional					
Saginaw Bay	2 Dimensional Laterally	5	8	Chlorophyll, Zooplankton, Phosphorus Nitrogen Silica	Week-Week and Year-Year	
Lake Erie	3 Dimensional					Includes sediment interactions
Chesapeake Bay	2 Dimensional Laterally	49	5	Chlorophyll, Nitrogen, Phosphorus	Steady State	Simplified eutrophication kinetics
Trinity River						
Tennessee Colony	2 Dimensional Vertically	15	7	Chlorophyll, Nitrogen, Phosphorus		
Lake Livingston	2 Dimensional	14	8	Chlorophyll, Nitrogen Phosphorus		
Upper Mississippi	3 Dimensional	120	12	Chlorophyll, Nitrogen, Phosphorus, DO, Bacteria	Steady State	
Minneapolis 208						

TABLE 1. APPLICATIONS OF WASP PROGRAM (Continued)

Geographical Area	Spatial Dimensionality	Number of Spatial Segments	Number of State Variables	Principal State Variables	Time Scale	Remarks
Dissolved Oxygen, Bacteria Problem Contexts						
Upper Delaware River	1 Dimensional	120	3	BOD, DO	Hour-Hour	Included rooted aquatic plants
New York Harbor (208)	3 Dimensional	425	6	BOD, DO, Bacteria	Day-Day	Interfaced to landside simulator
Milwaukee River	1 Dimensional	67	3	BOD, DO, Bacteria	Hour-Hour	
Toxic Substance Problem Contexts						
Hudson River - NY Harbor PCB	1 Dimensional	21	3	Suspended solids, Dissolved PCBs, Particulate PCBs	Steady State	
Quarry - DDE and Lindane	1 Dimensional Vertically	15	5	Suspended solids, Dissolved and Particulate DDE and Lindane	Minute-Minute	
River - pH Spill	2 Dimensional Laterally	78	2	Bicarbonate equilibrium - pH	Minute-Minute	
Ocean Disposal - Acid Waste	2 Dimensional Vertically	120	1	Acid Waste	Minute-Minute	Included stratification due to thermocline

TABLE 1. APPLICATIONS OF WASP PROGRAM (Continued)

Geographical Area	Spatial Dimensionality	Number of Spatial Segments	Number of State Variables	Principal State Variables	Time Scale	Remarks
Biological Waste Treatment Problem Contexts						
Anaerobic Filter		20	12	COD, DO, pH, Organic Nitrogen	Steady State	3 Phases-Solids, Liquid, Gas
Trickling Filter		20	2	Substrate, DO	Steady State	1 or 2 reactors in series, recycle
Pure Oxygen		4	6	COD, DO, Nitrogen, pH	Steady State	Gas - Liquid phase

1.1 OVERVIEW OF THE WASP3 MODELING SYSTEM

The WASP3 system consists of two stand-alone computer programs, DYNHYD3 and WASP3, that can be run in conjunction or separately (Figure 1). The hydrodynamics program, DYNHYD3, simulates the movement of water while the water quality program simulates the movement and interaction of pollutants within the water. The latter program is supplied with two kinetic sub-models to simulate two of the major classes of water quality problems: conventional pollution (involving dissolved oxygen, biochemical oxygen demand, nutrients and eutrophication) and toxic pollution (involving organic chemicals or metals and sediment). The linkage of either sub-model with the WASP3 program gives the models EUTROWASP and TOXIWASP, respectively. This is illustrated in Figure 1 with blocks to be substituted into the incomplete WASP3 model. The tracer block is a dummy sub-model for substances with no kinetic interactions.

The basic principle of both the hydrodynamics and water-quality program is the conservation of mass. The water volume and water-quality constituent masses being studied are tracked and accounted for over time and space using a series of mass balancing equations. The hydrodynamics program also conserves momentum, or energy, throughout time and space.

1.2 THE HYDRODYNAMICS MODEL

1.2.1 Overview of DYNHYD3

The WASP3 hydrodynamics model DYNHYD3 is an enhancement of the Potomac Estuary hydrodynamic model DYNHYD2 (Roesch et al., 1979), which was a component of the Dynamic Estuary Model (Feigner and Harris, 1970). DYNHYD3 solves the one-dimensional equations of continuity and momentum for a branching or channel-junction (link-node), computational network. Driven by variable upstream flows and downstream heads, simulations typically proceed at 1- to 5-minute intervals. The resulting unsteady hydrodynamics are averaged over larger time intervals and stored for later use by the water-quality program.

1.2.2 The Hydrodynamic Equations

The hydrodynamic model solves one-dimensional equations describing the propagation of a long wave through a shallow water system while conserving both momentum (energy) and volume (mass). The equation of motion, based on the conservation of momentum, predicts water velocities and flows. The equation of continuity, based on the conservation of volume, predicts water heights (heads) and volumes. This approach assumes that flow is predominantly one-dimensional, that Coriolis and other accelerations normal to the direction of flow are negligible, that channels are rectangular with uniform cross-sectional area, that the wave length is significantly greater than the depth, and that bottom slopes are moderate.

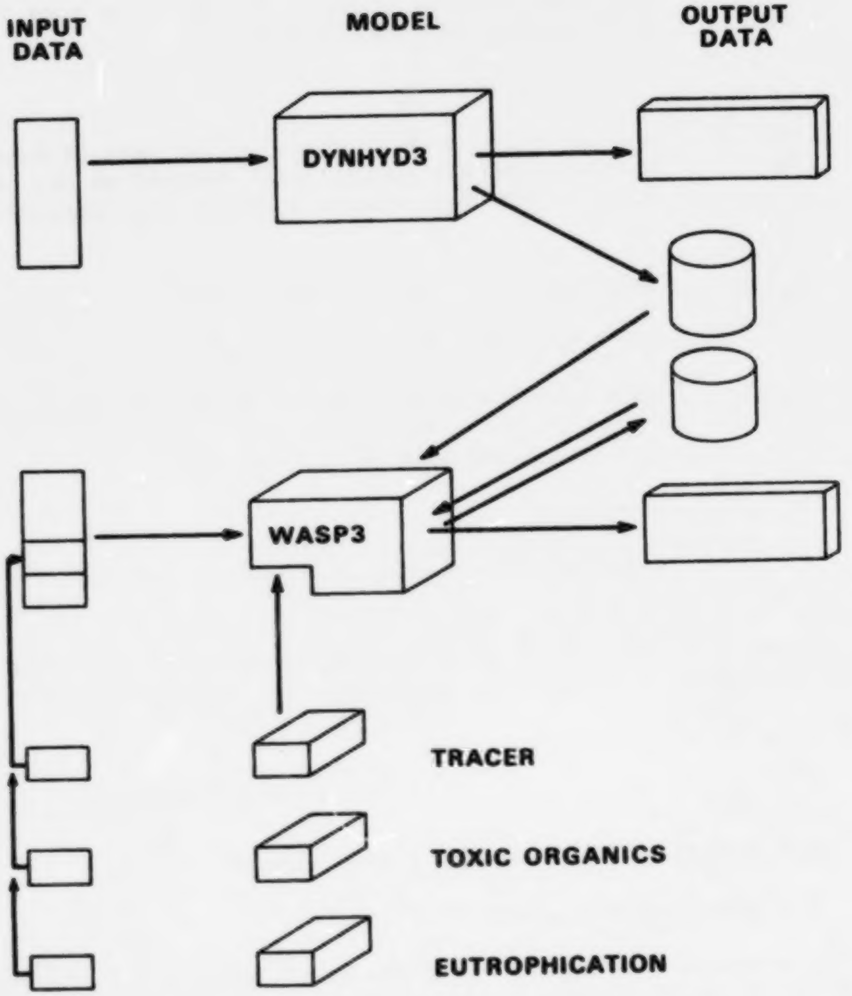

INPUT DATA
MODEL
OUTPUT DATA
DYNHYD3
WASP3
TRACER
TOXIC ORGANICS
EUTROPHICATION

Figure 1. The basic WASP system.

1.2.2.1 Equation of Motion

The equation of motion is given by:

$$\frac{\partial U}{\partial t} = - U \frac{\partial U}{\partial x} + a_{g,\ell} + a_f + a_{w,\ell} \qquad 1$$

where: $\frac{\partial U}{\partial t}$ = the local inertia term, or the velocity rate of change with respect to time, ft/sec^2

$U\frac{\partial U}{\partial x}$ = the Bernoulli acceleration, or the rate of momentum change by mass transfer; also defined as the convective inertia term from Newton's second law, ft/sec^2

$a_{g,\ell}$ = gravitational acceleration, ft/sec^2

a_f = frictional acceleration, ft/sec^2

$a_{w,\ell}$ = wind stress acceleration along axis of channel, ft/sec^2

x = distance along axis of channel, ft

t = time, sec

U = velocity along the axis of channel, ft/sec.

Gravitational acceleration is driven by the slope of the water surface. Referring to Figure 2, the acceleration along the longitudinal axis is

$$a_{g,\ell} = -g \cdot \sin S \qquad 2$$

where:

g = acceleration of gravity = 32.2 ft/sec^2

S = water surface slope, ft/ft.

Because the value of S is small, sin S can be replaced by S. Expressing S as the change of water surface elevation with longitudinal distance gives:

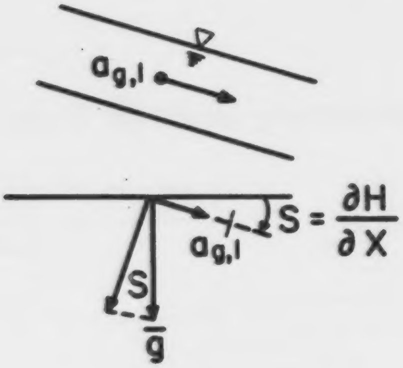
$$a_{g,\ell} = -g \cdot \frac{\partial H}{\partial x} \qquad 3$$

where:

H = water surface elevation, or head (height above an arbitrary datum), ft

The frictional acceleration term can be expressed using the Manning equation for steady uniform flow:

Acceleration of Gravity = g



$$a_{g,l} = -g \cdot \sin S \approx -g \cdot S$$

$$\boxed{a_{g,l} = -g \frac{\partial H}{\partial X}}$$

Figure 2. Gravitational acceleration.

$$U = -\frac{1.486\ R^{2/3}}{n} \cdot \frac{\partial H}{\partial x}^{1/2} \qquad 4$$

where:

R = hydraulic radius (approximately equal to the depth), ft

n = Manning roughness coefficient (usually between 0.01 and 0.10), sec.$m^{-1/3}$

$\frac{\partial H}{\partial x}$ = the energy gradient, ft/ft

1.486 = conversion factor, $ft^{1/3}.m^{-1/3}$

Referring to Figure 3, gravitational acceleration balances frictional resistance for steady flow conditions, such that:

$$a_f = -g \frac{\partial H}{\partial x} \qquad 5$$

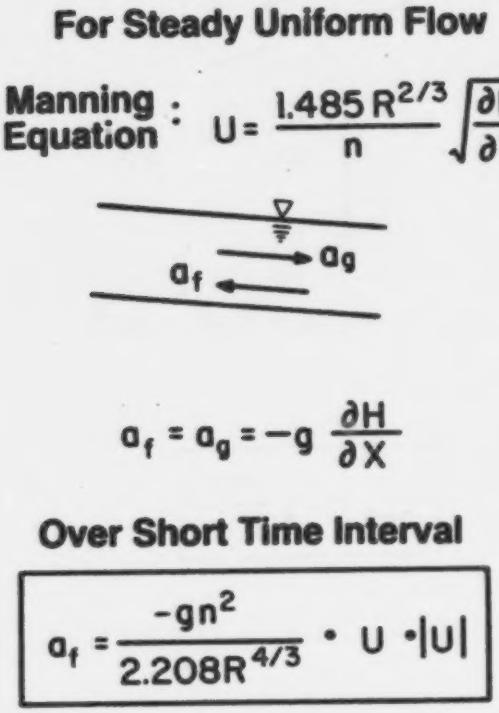

For Steady Uniform Flow
Manning Equation : $U = \frac{1.485\,R^{2/3}}{n}\sqrt{\frac{\partial H}{\partial X}}$
a_g
a_f
$a_f = a_g = -g\,\frac{\partial H}{\partial X}$
Over Short Time Interval
$a_f = \frac{-gn^2}{2.208R^{4/3}} \cdot U \cdot |U|$

Figure 3. Frictional acceleration.

Unfortunately, tidally influenced estuaries rarely experience truly steady flow. Over short time intervals, however, flow may be considered steady and uniform. Consequently, the energy gradient from equation 4 can be substituted into 5 to give:

$$a_f = -\frac{g\,n^2}{2.208\,R^{4/3}} \cdot U.|U| \qquad 6$$

where U^2 has been replaced by U times the absolute value of U so friction will always oppose the direction of flow.

Referring to Figure 4, the magnitude of the wind acceleration term can be derived from the shear stress equation at the air-water boundary:

$$\tau_w = C_d \rho_a W^2 \qquad 7$$

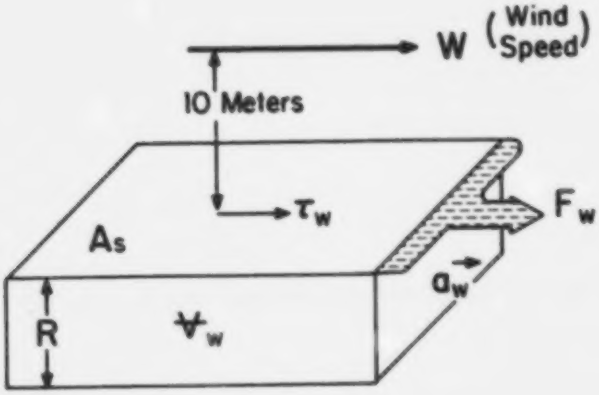
where:

τ_w = the boundary shear stress, $lb_m/ft\text{-}sec^2$

C_d = the drag coefficient (= 0.0026), unitless

ρ_a = the density of air, lb_m/ft^3

W = the wind speed (relative to the moving water surface) measured at a height of 10 meters, ft/sec



$$\tau_w = C_d \rho_a W^2$$

$$F_w = \tau_w \cdot A_s$$

$$a_w = F_w / (\forall_w \cdot \rho_w)$$

$$\boxed{a_w = \frac{C_d}{R} \frac{\rho_a}{\rho_w} W^2}$$

$$C_d = 0.0026$$

$$\rho_a / \rho_w = 1.165 \times 10^{-3}$$

Figure 4. Wind acceleration magnitude.

The force exerted on the water surface, A_s, is:

$$F_w = \tau_w \cdot A_s \qquad 8$$

Substituting equation 7 gives:

$$F_w = C_d \, A_s \, \rho_a \, W^2 \qquad 9$$

This force causes a volume of water V_w to accelerate in the wind direction:

$$a_w = \frac{F_w}{V_w \cdot \rho_w} \qquad 10$$

Substituting equation 9 gives the following equation for the wind acceleration term:

$$a_w = \frac{C_d}{R} \frac{\rho_a}{\rho_w} W^2 \qquad 11$$

where ρ_w = density of water, lb_m/ft^3

$$\frac{\rho_a}{\rho_w} = 1.165 \times 10^{-3}$$

The hydraulic radius, R, is equal to the volume divided by the cross-sectional area:

$$R = V_w/A_s \qquad 12$$

where: A_s = surface area, ft^2

V_w = water volume, ft^3

Referring to Figure 5, the component of acceleration along the channel axis is:

$$a_{w,\ell} = \frac{C_d}{R} \frac{\rho_a}{\rho_w} W^2 \cos \Psi \qquad 13$$

where Ψ = the angle between the channel direction and the wind direction (relative to the moving water surface)

Both the water and wind have velocity components that contain both magnitude and direction. If the water is moving with a velocity $\underline{U}$, then the wind velocity $\overline{W}$ experienced at the water surface is given by the following (see Figure 6):

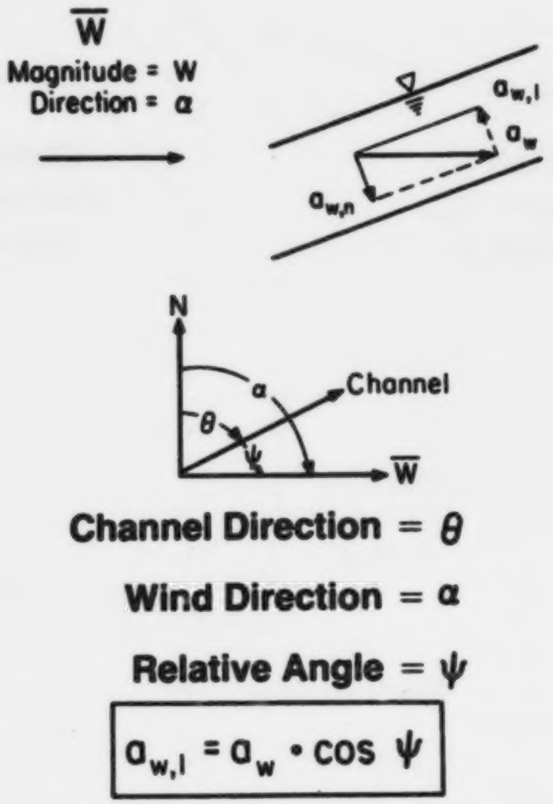

W̄
Magnitude = W
Direction = α
$a_{w,l}$
a_w
$a_{w,n}$
N
α
Channel
θ
ψ
W̄
Channel Direction = θ
Wind Direction = α
Relative Angle = ψ
$a_{w,l} = a_w \cdot \cos\psi$

Figure 5. Wind stress direction.

$$\overline{W} = \overline{W}_{obs} - \overline{U} \qquad 14$$

where:

$\overline{W}_{obs}$ = the wind velocity observed at a stationary location, 32.2 ft (10 meters) above the water surface (magnitude = W_{obs}, direction = ϕ)

$\overline{U}$ = the water velocity (magnitude = U, direction = θ)

Therefore, $\overline{W}$ is the relative wind velocity with magnitude W, and the effective wind angle relative to the channel axis is

$$\Psi = \alpha - \Theta \qquad 15$$

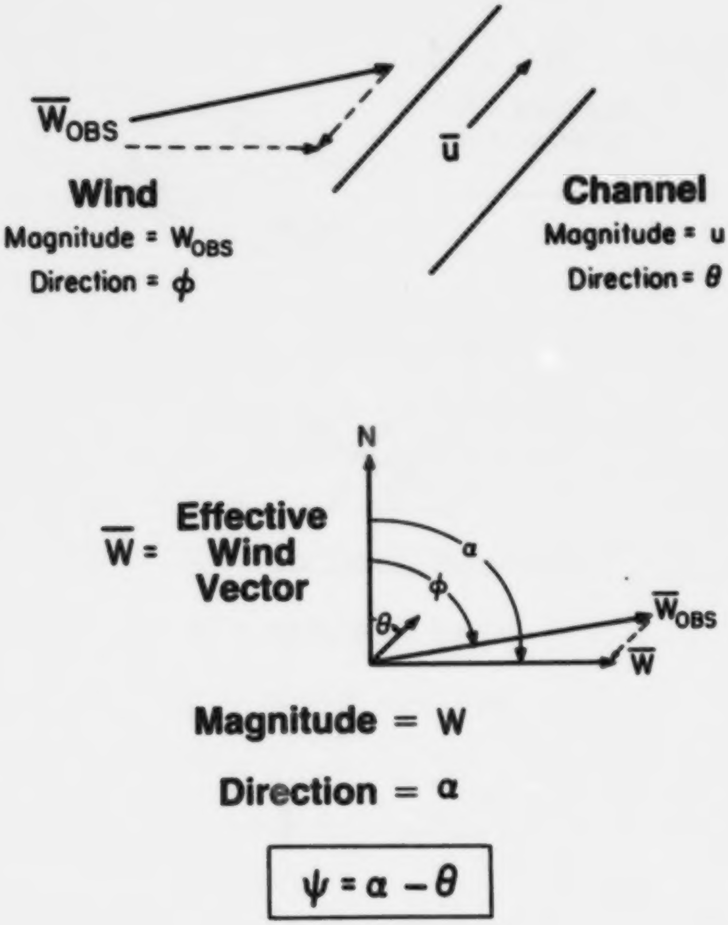

$\overline{W}_{OBS}$
$\overline{u}$
Wind
Magnitude = W_{OBS}
Direction = ϕ
Channel
Magnitude = u
Direction = θ
N
$\overline{W}$ = Effective Wind Vector
α
ϕ
θ
$\overline{W}_{OBS}$
$\overline{W}$
Magnitude = W
Direction = α
$\psi = \alpha - \theta$

Figure 6. Wind stress.

Given observations of W_{obs}, U, ϕ, and θ, the magnitude and direction of W can be calculated using vector analysis (Figure 7):

$$W^2 = U^2 + W_{obs}^2 - 2.U.W_{obs}.\cos(\theta - \phi) \qquad 16$$

$$\alpha = \tan^{-1}\left[\frac{W_{obs} \sin\phi - U \sin\theta}{W_{obs} \cos\phi - U \cos\theta}\right] \qquad 17$$

Wind acceleration can either enhance or oppose stream flow, depending on the relative direction of the wind ψ. For wind blowing normal to the channel axis, $\cos \psi = 0$, and there is no acceleration along the axis. For wind blowing along the axis in a positive direction, $\cos \psi = +1$. Positive flow in the channel will be enhanced, and negative flow will be opposed.

Vector	X	Y
U	$U \sin\theta$	$U \cos\theta$
W_{OBS}	$W_{OBS} \sin\phi$	$W_{OBS} \cos\phi$
W	$W_{OBS} \sin\phi - U \sin\phi$	$W_{OBS} \cos\phi - U \cos\theta$

$$\boxed{\begin{array}{l} W^2 = U^2 + W_{OBS}^2 - \partial U \, W_{OBS} \bullet \cos(\theta - \phi) \\ \partial = \tan^{-1}\left[\dfrac{W_{OBS} \sin\phi - U \sin\theta}{W_{OBS} \cos\phi - U \cos\theta}\right] \\ \psi = \alpha - \theta \end{array}}$$

Figure 7. Wind stress vector analysis.

Conversely, for wind blowing along the axis in a negative direction, $\cos \Psi = -1$. Positive flow in the channel will be opposed, and negative flow will be enhanced (refer to Figure 8).

Wind and Stream Directions	ψ	$\cos \psi$	Effect
W→ |U↑|	90°	0	None
W→ U→	0°	1	Enhanced Acceleration
W→ ←U	180°	-1	Opposed
←W U→	180°	-1	Opposed
←W ←U	0°	1	Enhanced

Figure 8. Wind stress effects.

1.2.2.2 Equation of Continuity

The equation of continuity is given by:

$$\frac{\partial A}{\partial t} = -\frac{\partial Q}{\partial x} \qquad 18$$

where:

A = cross-sectional area, ft^2

Q = flow, ft^3/sec

For rectangular channels of constant width b (refer to Figure 9):

$$\frac{\partial H}{\partial t} = -\frac{1}{b} \cdot \frac{\partial Q}{\partial x} \qquad 19$$

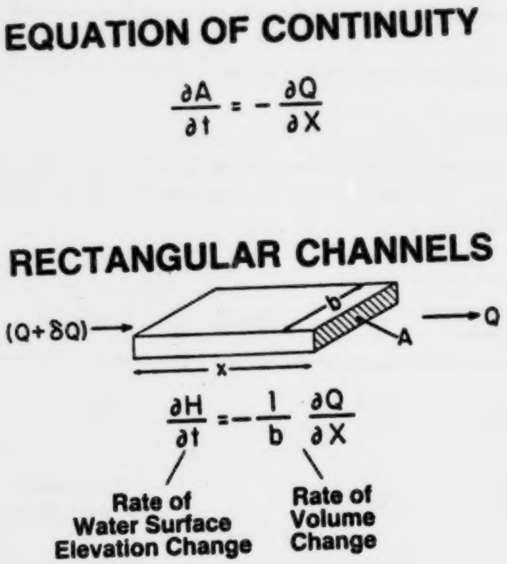

EQUATION OF CONTINUITY
$\frac{\partial A}{\partial t} = -\frac{\partial Q}{\partial X}$
RECTANGULAR CHANNELS
(Q+δQ)
b
A
Q
x
$\frac{\partial H}{\partial t} = -\frac{1}{b}\frac{\partial Q}{\partial X}$
Rate of Water Surface Elevation Change
Rate of Volume Change

Figure 9. Equation of continuity.

where:

b = width, ft

H = water surface elevation (head), ft

$\frac{\partial H}{\partial t}$ = rate of water surface elevational change with respect to time, ft/sec

$\frac{1}{b} \cdot \frac{\partial Q}{\partial x}$ = rate of water volume change with respect to distance per unit width, ft/sec

1.2.3 The Model Network

Equations 1 and 19 form the basis of the hydrodynamic model DYNHYD3. Their solution gives velocities (U) and heads (H) throughout the water body over the duration of the simulation. Because closed-form analytical solutions are unavailable, the solution of equations 1 and 19 requires numerical integration on a computational network, where values of U and H are calculated at discrete points in space and time.

A flexible, computationally efficient type of network has been developed for these equations (Feigner and Harris, 1970). The "link-node" network solves the equations of motion and continuity at alternating grid points. At each time step, the equation of motion is solved at the links, giving velocities for mass transport calculations, and the equation of continuity is solved at the nodes, giving heads for pollutant concentration calculations (Figure 10).

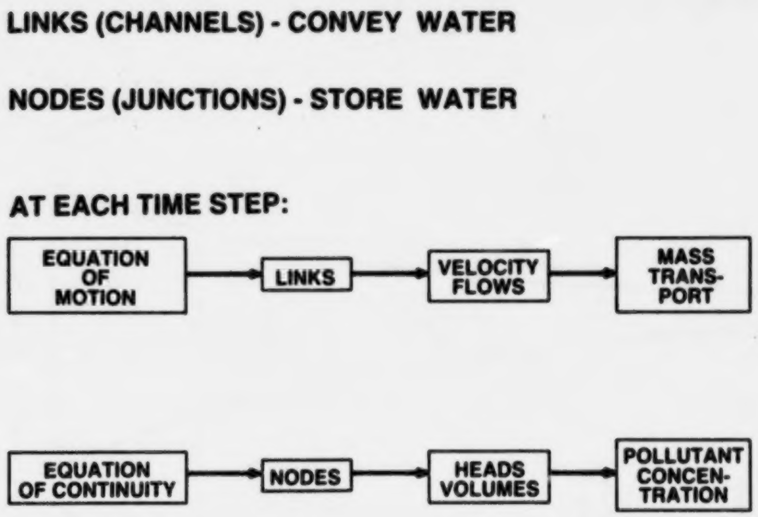
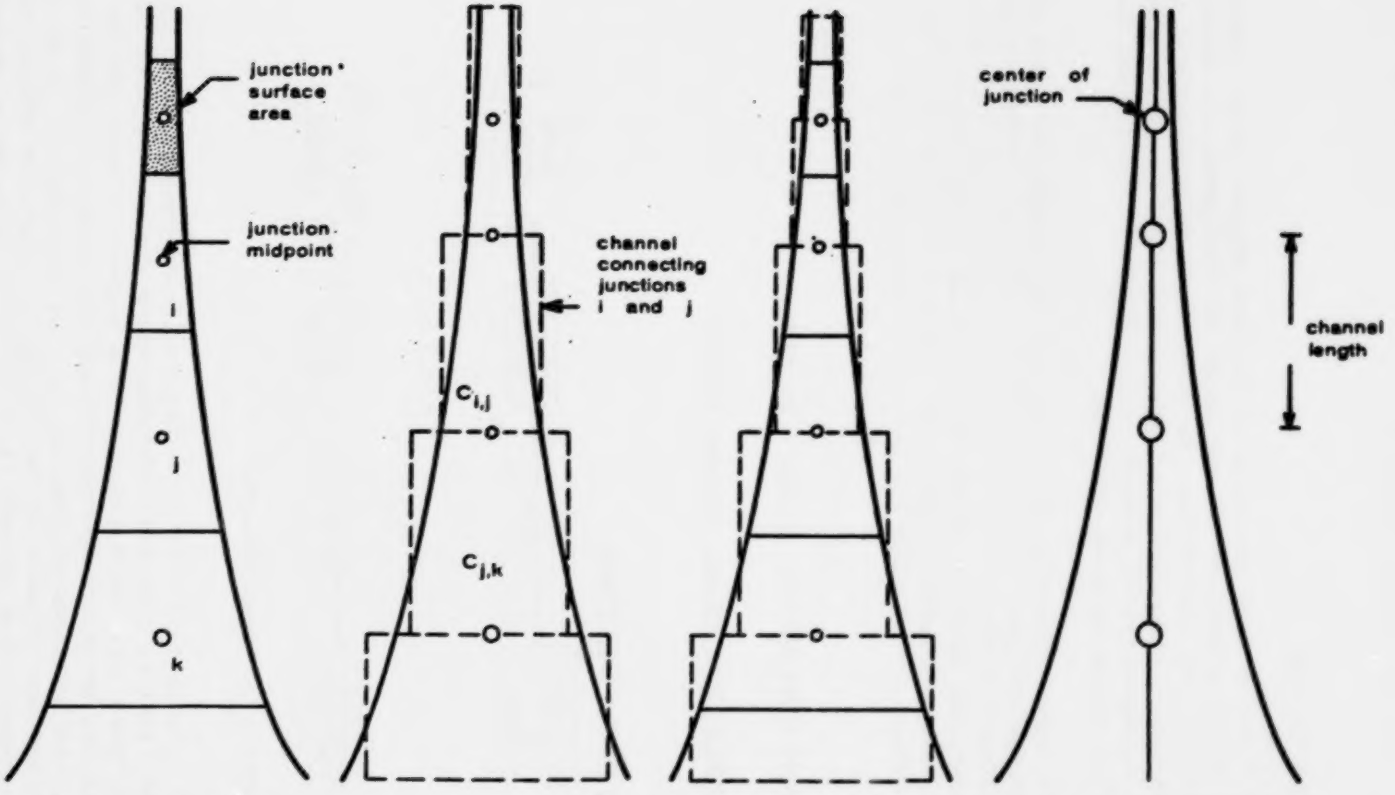

LINKS (CHANNELS) - CONVEY WATER
NODES (JUNCTIONS) - STORE WATER
AT EACH TIME STEP:
EQUATION OF MOTION
LINKS
VELOCITY FLOWS
MASS TRANS-PORT
EQUATION OF CONTINUITY
NODES
HEADS VOLUMES
POLLUTANT CONCEN-TRATION

Figure 10. Model network.

A physical interpretation of this computational network can be developed by picturing the links as channels conveying water and the nodes as junctions storing water (Figure 11). Each junction is a volumetric unit that acts as a receptacle for the water transported through its connecting channels. Taken together, the junctions account for all the water volume in the river or estuary. Parameters influencing the storage of water are defined within this junction network. Each channel is an idealized rectangular conveyor that transports water between two junctions, whose midpoints are at each end.


junction surface area
junction midpoint
i
j
k
channel connecting junctions i and j
$C_{i,j}$
$C_{j,k}$
center of junction
channel length

(b) Junction Network (a) Channel Network (c) Model Network (d) Network Representation

Figure 11. Representation of the model network.

Taken together, the channels account for all the water movement in the river or estuary. Parameters influencing the motion of water are defined within this channel network. The link-node computational network, then, can be viewed as the overlapping of two closely related physical networks of channels and junctions.

Junctions are equivalent to segments in the water quality model, whereas channels correspond to segment interfaces. Channel flows are used to calculate mass transport between segments in the water quality model. Junction volumes are used to calculate pollutant concentrations within water quality segments.

Link-node networks can treat fairly complex branching flow patterns and irregular shorelines with acceptable accuracy for many studies. They cannot handle stratified water bodies, small stream, or rivers with a large bottom slope. Link-node networks can be set up for wide, shallow water bodies if primary flow directions are well defined. Results of these simulations should be considered descriptive only.

1.2.4 Implementation of the Equations

To apply differential equations 1 and 19 to a link-node computational network, they must first be written in a finite difference form. The equation of motion becomes:

$$\frac{U_i^t - U_i}{\Delta t} = -U_i \frac{\Delta U_i}{\Delta x_i} - g \frac{\Delta H_i}{\Delta x_i} - \frac{g\, n_i^2}{2.208 R_i^{4/3}} \cdot U_i |U_i| + \frac{C_d}{R_i} \frac{\rho_a}{\rho_w} \cdot W_i^2 \cdot \cos \Psi_i \qquad 20$$

where: U_i^t = the velocity in channel i at time t, ft/sec

Δx_i = the channel length, ft

Δt = the time step, sec

i = channel or link number

$\frac{\Delta U_i}{\Delta x_i}$ = velocity gradient in channel i with respect to distance, sec^{-1}

$\frac{\Delta H_i}{\Delta x_i}$ = water surface gradient in channel i with respect to distance, ft/ft

All values on the right hand side of equation 20 are referenced to the previous time step (t-1).

The water surface gradient, $\Delta H_i/\Delta x_i$, can be computed from the junction heads at either end of the channel. The velocity gradient, however, cannot be computed directly from upstream and downstream channel velocities because of possible branching in the network. If branching does occur, there would be several upstream and downstream channels, and any computed velocity gradient would be ambiguous. An expression for the velocity gradient within a channel can be derived by applying the continuity equation 18 to the channel and substituting U . A for Q:

$$\frac{\partial A}{\partial t} = -\frac{\partial Q}{\partial x} = -U\frac{\partial A}{\partial x} - A\frac{\partial U}{\partial x} \qquad 21$$

Rearranging terms:

$$\frac{\partial U}{\partial x} = -\frac{1}{A}\left(\frac{\partial A}{\partial t}\right) - \frac{U}{A}\cdot\left(\frac{\partial A}{\partial x}\right) \qquad 22$$

Writing this in finite difference form and substituting b.R for A and b.ΔH for ∂A gives the following expression for the velocity gradient:

$$\frac{\Delta U_i}{\Delta x_i} = -\frac{1}{R_i}\frac{\Delta H_i}{\Delta t} - \frac{U_i}{R_i}\frac{\Delta H_i}{\Delta x_i} \qquad 23$$

The term $\Delta H_i/\Delta t$ is computed as the average water surface elevational change between the junctions at each end of channel i during time step t. Substituting equation 23 into 20 and rearranging gives the explicit finite difference equation of motion applied to each channel i:

$$U_i^t = U_i + \Delta t\,[\frac{U_i}{R_i}\frac{\Delta H_i}{\Delta t} + (\frac{U_i^2}{R_i} - g)\frac{\Delta H_i}{\Delta x_i}$$

$$- \frac{g\,n_i^2}{2.208R_i^{4/3}}\cdot U_i|U_i| + \frac{C_d}{R_i}\frac{\rho_a}{\rho_w}W_i^2\cdot\cos\Psi_i] \qquad 24$$

Writing the equation of continuity (19) in finite difference form gives:

$$\frac{H_j^t - H_j}{\Delta t} = -\frac{\Delta Q_j}{b_j\cdot\Delta x_j} \qquad 25$$

The numerator ΔQ_j is given by the summation of all flows entering and leaving the junction. The denominator $b_j.\Delta x_j$ can be expressed directly as the surface area A_j^s of the junction. Substituting these identities into equation 25 and rearranging gives the explicit finite difference equation of continuity applied to each junction j:

$$H_j^t = H_j - \Delta t \cdot \left[\frac{\sum_i Q_{ij}}{A_j^s} \right] \qquad 26$$

At this point, one equation for each channel and each junction in the computational network exists. Given input parameters describing the network configuration and geometry, initial values for channel velocities and junction heads, boundary conditions for downstream heads, and forcing functions for freshwater inflow and wind stress, equations 24 and 26 are solved using a modified Runge-Kutta procedure. The solution proceeds in eight steps, which are repeated throughout the simulation:

1) For the middle of the next time interval (i.e., for time t + Δt/2), the mean velocity for each channel is predicted using the channel velocities and cross-sectional areas and the junction heads at the beginning of the current time interval.

2) For t + Δt/2, the flow in each channel is computed using the velocity obtained in step (1) and the cross-sectional area at the beginning of the current interval.

3) At t + Δt/2, the head at each junction is computed using the flows derived in step (2).

4) At t + Δt/2, the cross-sectional area of each channel is computed using the heads computed in step (3).

5) The mean velocity for each channel is predicted for the full time step (t + Δt) using the velocities, cross-sectional areas, and junction heads computed for t + Δt/2 in steps (1), (3), and (4).

6) The flow in each channel for t + Δt is computed using the velocity for the full time step (computed in step 5) and the cross-sectional area computed for t + Δt/2 in step (4).

7) The head at each junction after t + Δt is computed using the full step flow computed in step (6).

8) The cross-sectional area of each channel after a full time step is computed using the full step heads from step (7).

9) Repeat steps (1) through (8) for the specified number of time intervals.

1.2.5 The Model Parameters

This section summarizes the input parameters that must be specified in order to solve the equations of motion and continuity. Other parameters calculated by the model also are discussed.

1.2.5.1 Junction Parameters

The input parameters associated with junctions are initial surface elevation (head), surface area, and bottom elevation. Volumes and mean depths are calculated internally. A definition sketch is given in Figure 12.

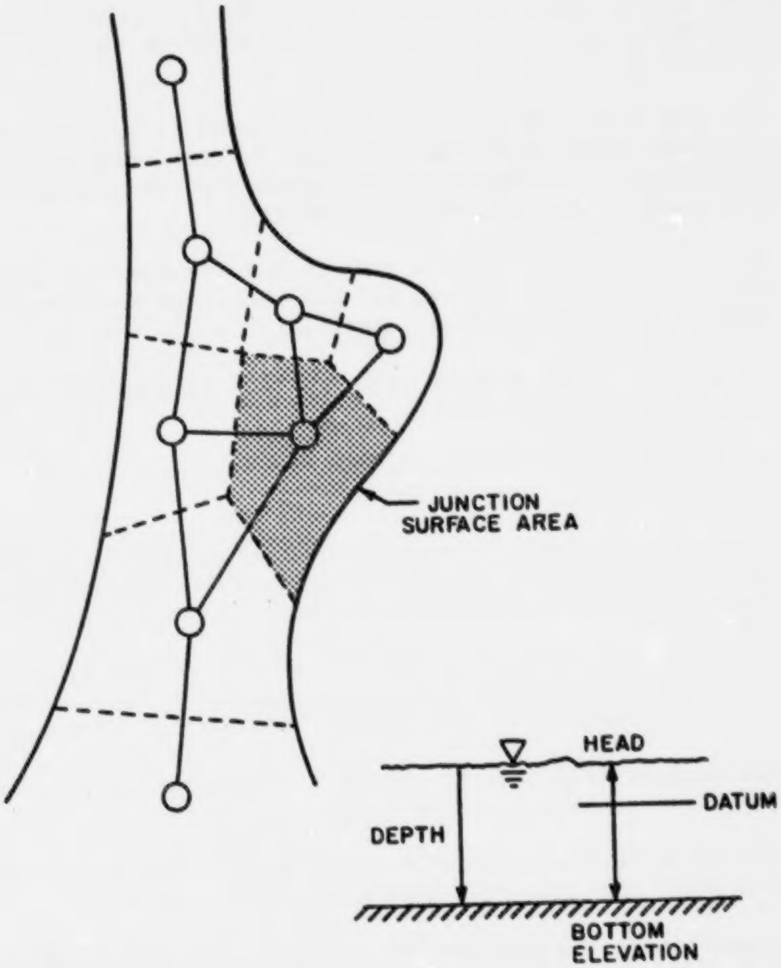

JUNCTION SURFACE AREA
HEAD
DATUM
DEPTH
BOTTOM ELEVATION

Figure 12. Definition sketch of junctions.

Surface elevation or head, ft--Junction heads represent the mean elevation of the water surface above or below an arbitrary horizontal datum. The datum is usually the mean local sea level. If initial surface elevations are not input, they will be calculated from bottom elevation and depth.

Surface area, ft^2--Except when branching or looping occurs (i.e., when more than two channels enter a junction), the surface area of a junction is equated to one-half of the sum of the surface areas of the two channels entering the junction. When branching or looping does occur, the junction surface areas can be determined by laying out a polygon network using the Thiessen Polygon method, as in Figure 12. Since the polygons are normally irregular, a planimeter must be used to obtain the surface areas.

Bottom elevation, ft--The mean elevation of the junction bottom above or below the datum is defined as the bottom elevation. If initial surface elevations are specified, bottom elevations will be calculated internally by subtracting the mean depth from the mean head.

Volume, ft^2--Initial junction volumes are computed internally by multiplying the junction surface area by the mean depth of the channels (weighted by their cross-sectional area) entering the junction. Junction volumes are updated throughout the simulation by adding the product of the surface area and the change in surface elevation to the initial volume.

1.2.5.2 Channel Parameters

The input parameters associated with channels are length, width, hydraulic radius or depth, channel orientation, initial velocity, and Manning's roughness coefficient. A definition sketch is given in Figure 13.

Length, ft--The channel length is the distance between the midpoints of the two junctions it connects. Channels must be rectangular and should be oriented so as to minimize the depth variation as well as reflect the location and position of the actual prototype channels. The channel length is generally dependent on a computational stability criteria given by:

$$\ell_i \geq (\sqrt{gy_i} \pm U_i)\ \Delta t \tag{27}$$

where:

ℓ_i = length of channel i, ft

y_i = mean depth of channel i, ft

U_i = velocity in channel i, ft/sec

Δt = computational time step

g = acceleration of gravity

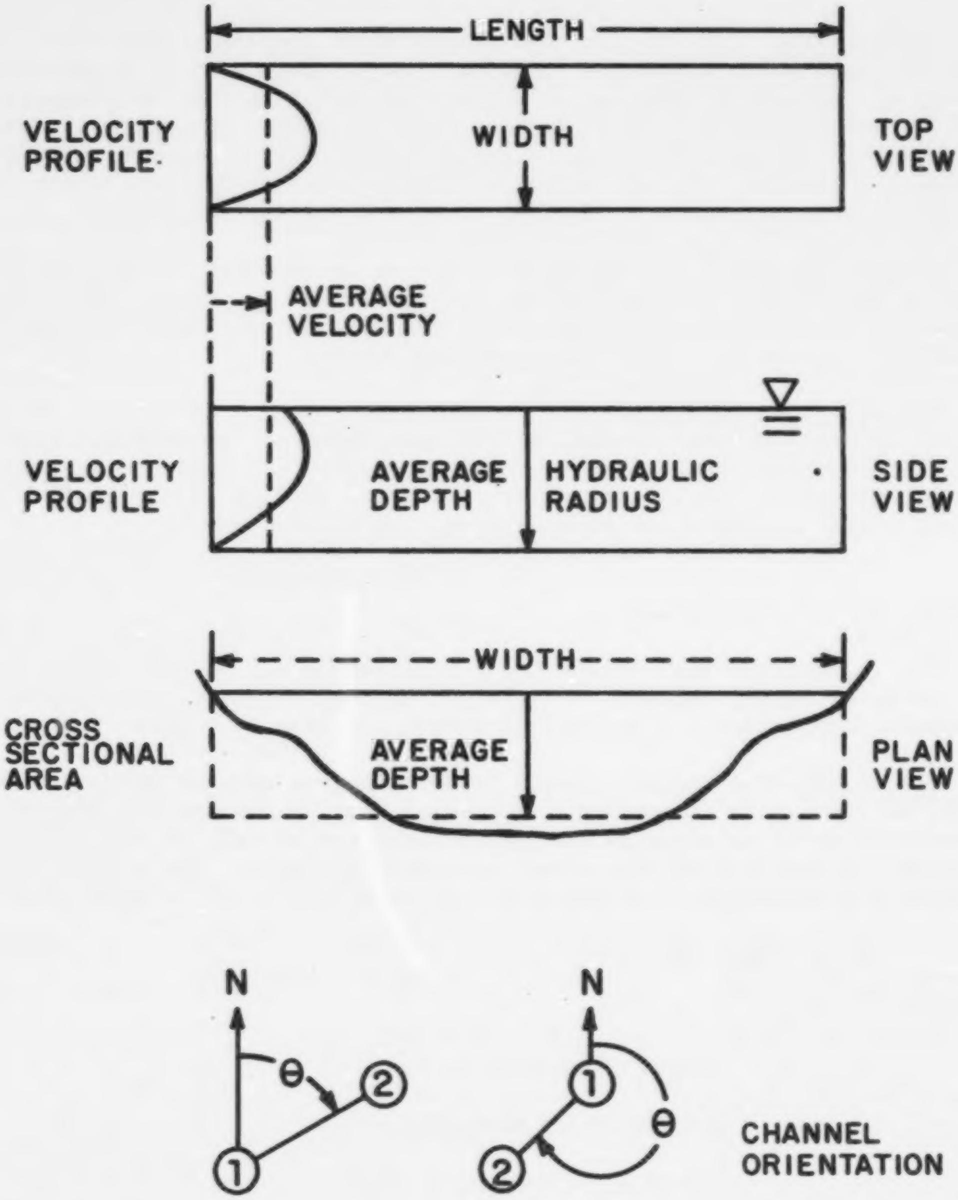

LENGTH
VELOCITY PROFILE
WIDTH
TOP VIEW
AVERAGE VELOCITY
VELOCITY PROFILE
AVERAGE DEPTH
HYDRAULIC RADIUS
SIDE VIEW
WIDTH
CROSS SECTIONAL AREA
AVERAGE DEPTH
PLAN VIEW
N
θ
①
②
N
①
②
θ
CHANNEL ORIENTATION

Figure 13. Definition sketch for channels.

Width, ft--There is no apparent limit on the width of a channel. If a channel is too wide in relation to its length, however, the mean velocity predicted may mask important velocity patterns occurring on a more local scale. For well defined channels, the network channel widths are equated to the average bank to bank width.

Cross-sectional area, ft^2--The cross-sectional area of a channel is equal to the product of the channel width and depth. Depth, however, is a channel parameter that must be defined with respect to junction head or water surface elevation (since both vary similarly with time). Initial values of width and depth based on the initial junction heads and the initial cross-sectional areas are computed internally. As the junction heads vary, the channel cross-sectional areas are adjusted accordingly.

Roughness--Channels are assigned "typical" Manning Roughness coefficients. The value of this coefficient should usually lie between 0.01 and 0.08. Because this parameter cannot be measured, it serves as a "knob" for the calibration of the model.

Velocity, ft/sec--An initial estimate of the mean channel velocity is required. Although any value may be assigned, the computational time required for convergence to an accurate solution will depend on how close the initial estimate is to the true value.

Hydraulic radius, ft--Previous applications of DYNHYD have used channels whose widths are greater than ten times the channel depth. Consequently, the hydraulic radius is usually assumed to be equal to the mean channel depth.

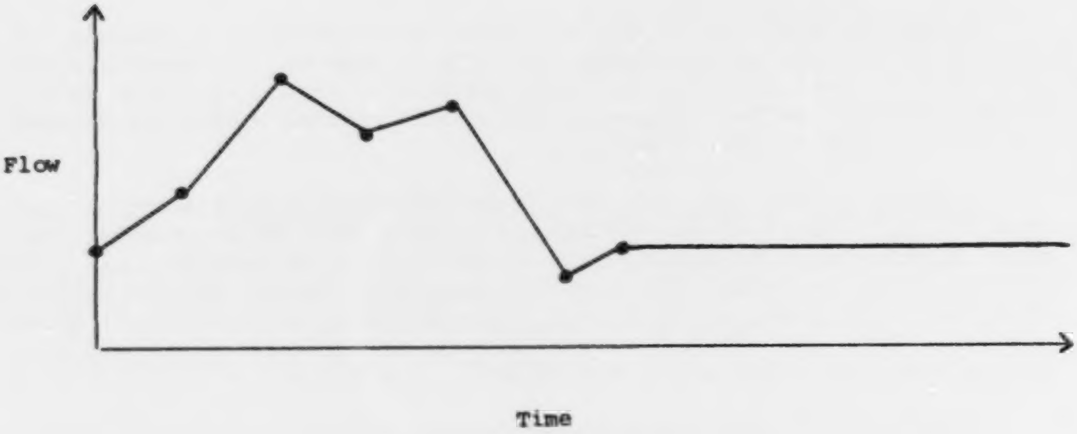
Channel orientation, degrees--The channel orientation is the direction of the channel axis measured from true north. The axis is assumed to point from lower junction number to higher junction number, which by convention, is the direction of positive flow.

1.2.5.3 Inflow Parameters

Inflows can be specified as constant or time variable. Inflows are represented by negative flows; outflows are represented by positive flows. For each time-variable inflow, a piecewise linear function of flow versus time is specified, as in Figure 14. If the simulation extends beyond the last specified flow, the flow assumes a constant inflow equal to the last specified flow.

1.2.5.4 Downstream Boundary Parameters

The downstream boundaries can be defined by either specifying outflows or surface elevations (tidal function). Outflows are handled as negative inflows, as discussed above. Surface elevations at each downstream boundary can be specified by an average tidal function or by a variable tidal function. A definition sketch is provided in Figure 15.



Piecewise Linear Function

Day	Time Hour:Min	Flow ft^3/sec
1	09 30	30.
2	10 00	40.
3	13 00	80.
4	12 30	70.
5	12 00	75.
6	18 30	20.
7	09 30	30

Figure 14 Inflow Time Function

Average tidal function: For some simulations, the average tidal variability will produce accurate predictions of tidal transport. Tidal heights (referenced to the model datum) are specified at equally spaced intervals throughout the average tidal cycle. Normally, 30-minute intervals will suffice. These data can be obtained from tidal stage recorders located at or near the model boundary. If no recorders are available, the predictions presented in the U.S. Coast and Geodetic Survey Tide Tables can be used.

DYNHYD3 reduces the height versus time data to the following function using the subroutine REGAN.

$$y = A_1 + A_2\sin(\omega t)+A_3\sin(2\omega t)+A_4\sin(3\omega t) + A_5\cos(\omega t)+A_6\cos(2\omega t)+A_7\cos(3\omega t) \quad 28$$

where: y = tidal elevation above or below the model datum, ft
A_i = regression coefficients, ft

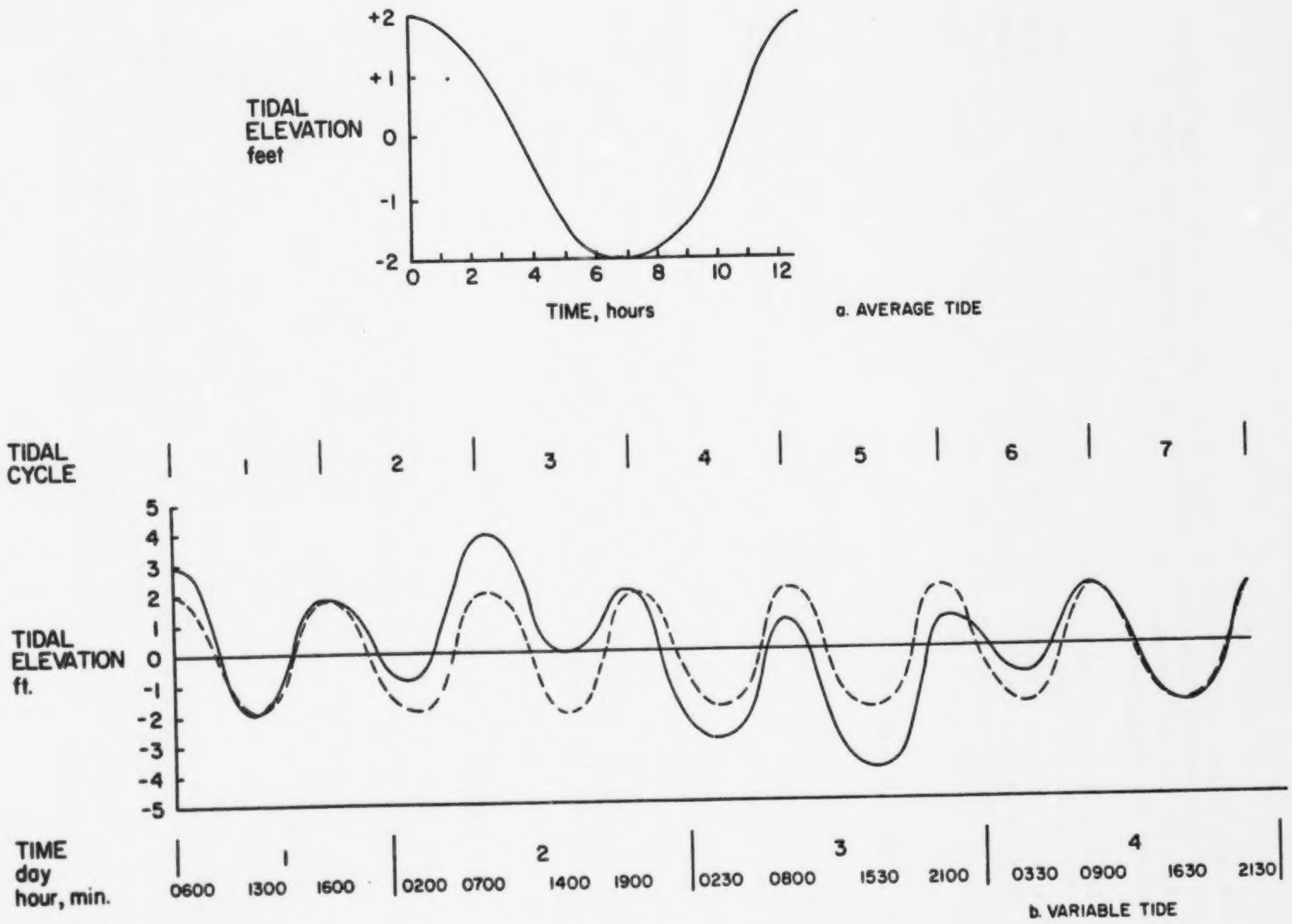


Figure 15. Definition sketch of downstream boundary.

ω = 2π/tidal period, hr^{-1}

t = time, hr

If the regression coefficients A_i are known, they can be specified instead of the height versus time data. All seven of the coefficients must be specified in the above order. The average tidal function is repeated throughout the simulation.

If data are available, variable tide patterns may be simulated by specifying the highs and lows of each tidal cycle. In this case, the subroutine RUNKUT will compute a sinusoidal curve between the data points. If simulation extends beyond the tidal cycle, the cycle will repeat. To insure this repetition, an odd number of data points must be specified with the last data point equal to the first.

1.2.5.5 Wind Parameters

The input parameters associated with wind acceleration are wind speed, wind direction, channel orientation, and channel hydraulic radius. The last two were discussed as channel parameters. A definition sketch was provided in Figure 12.

Wind speed (ft/sec) and direction (degrees from true north) are measured at a point 10 meters above the water surface. This wind is to be representative for the entire water body. Values of wind speed and direction can vary with time. Piecewise linear functions of wind speed and direction versus time are specified (similar to Figure 14 for flow). If the simulation extends beyond the last specified wind, the piecewise linear functions are repeated.

1.2.6 Application of the Model

A great deal of flexibility is allowed in laying out the network of interconnected channels and junctions that represent a system, but there are several guidelines for making the best representation. First, both hydraulic and quality factors should be considered when selecting boundary conditions. Ideally, the downstream boundary should extend to a flow gage, a dam, or the ocean. The upstream boundary should extend to or beyond the limits of any backwater or tidal effects on the inflowing streams. Such a network eliminates problems associated with dynamic boundary conditions, such as changing salinity or other quality conditions, which could be present if an inland point were chosen for the seaward boundary. Other considerations influencing boundary locations and the size of network elements include the location of specific points where quality predictions are required, the location of existing or planned sampling stations (and the availability of data for verification), the degree of network detail desired, and the computer time available for solution.

In most applications of DYNHYD3, Manning's roughness coefficient (n) will be the primary calibration parameter. The value of n can be highly variable, depending on such factors as bed roughness, vegetation, channel irregularities in cross-section or shape, obstructions, and depth. Values of n can potentially vary from less than 0.01 to greater than 0.08. For the larger rivers, reservoirs, and estuaries to which DYNHYD3 can be applied, however, values will usually fall between 0.01 and 0.04. Deeper, straighter reaches have lower roughness coefficients. In general, the value of n increases upstream as channels become more constricted and shallow.

When calibrating DYNHYD3, changing the value of n in one channel affects both upstream and downstream channels. Increasing n causes more energy to be dissipated in that channel. As a result, the height of a tidal or flood wave will decrease and the time of travel through the channel will increase. Lowering n decreases the resistance to flow, resulting in a higher tidal or flood wave and a shorter time of travel.

If the hydrodynamic results generated by a DYNHYD3 simulation are to be stored for use by WASP3, then both the networks and the time steps must be compatible (though not identical). Every DYNHYD3 junction must coincide exactly with a WASP3 segment. WASP3 may have additional segments not represented by junctions. For example, WASP3 benthic segments will have no corresponding junctions. Junction numbering need not correspond to segment numbering. Junction to segment mapping is specified in the WASP3 input data set. The WASP3 time step must be an even multiple of the DYNHYD3 time step. The ratio of time steps must be specified in the DYNHYD3 input data set. Typical ratios are between 6 and 30. Segmentation and time steps for WASP3 are discussed in the next section.

1.3 THE BASIC WATER QUALITY MODEL

WASP3 is a dynamic compartment model that can be used to analyze a variety of water quality problems in such diverse water bodies as ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters. This section presents the basic water quality model used to simulate dissolved, conservative chemicals, such as chlorides or dye tracer.

1.3.1 Overview of WASP3

The equations solved by WASP3 are based on the key principle of the conservation of mass. This principle requires that the mass of each water quality constituent being investigated must be accounted for in one way or another. WASP3 traces each water quality constituent from the point of spatial and temporal input to its final point of export, conserving mass in space and time.

To perform these mass balance computations, the user must supply WASP3 with input data defining seven important characteristics:

- model segmentation
- advective and dispersive transport
- boundary concentrations
- point and diffuse source waste loads
- kinetic parameters, constants, and time functions
- initial concentrations
- simulation and output control

These input data, together with the general WASP3 mass balance equations and the specific chemical kinetics equations, uniquely define a special set of water quality equations. These are numerically integrated by WASP3 as the simulation proceeds in time. At user-specified print intervals, WASP3 saves the values of all display variables for subsequent retrieval by post-processor subroutines. These routines produce tables, time plots, and spatial plots of variables specified by the user.

1.3.2 The General Mass Balance Equation

A mass balance equation for constituents in a body of water must account for all the material entering and leaving through direct and diffuse loading; advective and dispersive transport; and physical, chemical, and biological transformation. Consider the coordinate system shown in Figure 16, where the x- and y-coordinates are in the horizontal plane, and the z-coordinate is in the vertical plane. The mass balance equation around an infinitesimally small fluid volume is:

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(U_x \cdot C) - \frac{\partial}{\partial y}(U_y \cdot C) - \frac{\partial}{\partial z}(U_z \cdot C)$$

$$+ \frac{\partial}{\partial x}\left(E_x \cdot \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \cdot \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \cdot \frac{\partial C}{\partial z}\right)$$

$$+ S_L + S_B + S_K \qquad 29$$

where:

C = concentration of the water quality constituent, M/L^3

t = time, T

U_x, U_y, U_z = longitudinal, lateral, and vertical advective velocities, L/T

E_x, E_y, E_z = longitudinal, lateral, and vertical diffusion coefficients, L^2/T

S_L = direct and diffuse loading rate, $M/L^3/T$

WATER QUALITY EQUATION

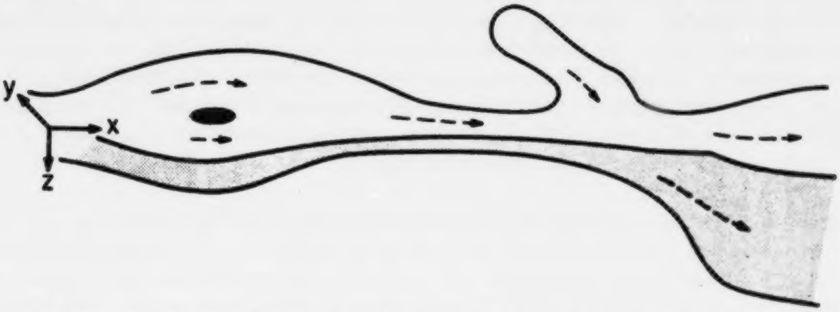


Figure 16. Coordinate system for mass balance equation.

S_B = boundary loading rate (including upstream, downstream, benthic, and atmospheric), $M/L^3/T$

S_K = total kinetic transformation rate; positive is source, negative is sink, $M/L^3/T$

L = length

M = mass

T = time

By expanding the infinitesimally small control volumes into larger adjoining "segments," and by specifying proper transport, loading, and transformation parameters, WASP implements a finite-difference form of equation 29. For brevity and clarity, however, the derivation of the finite-difference form of the mass balance equation will be for a one-dimensional reach. Assuming vertical and lateral homogeneity, we can integrate equation 29 over y and z to obtain

$$\frac{\partial}{\partial t}(A.C) = \frac{\partial}{\partial x}\left(-U_x \cdot A \cdot C + E_x \cdot A \cdot \frac{\partial C}{\partial x}\right) + A \cdot (S_L+S_B) + A \cdot S_K \qquad 30$$

where:

A = cross-sectional area, L^2

This equation represents the three major classes of water quality processes--transport (term 1), loading (term 2), and transformation (term 3).

Transport includes advective flow and dispersive mixing, which move the water quality constituents within a water body. Advective flow carries the water quality constituents "downstream" with the water and accounts for instream dilution (advective flows may reverse direction in estuaries due to tide, in lakes due to wind, or in rivers due to backwater). Dispersion causes further mixing and dilution of the water quality constituents as they move from regions of high concentration to regions of low concentration. In rivers, dispersion causes exchange between the main channel and any side embayments. In reservoirs and lakes, dispersion also causes mixing between surface and bottom-waters. In estuaries, dispersion also causes additional upstream tidal and density-driven mixing.

Loading includes both direct external input of pollutants to the water body and indirect interaction with the boundaries. While external inputs of pollutants are primarily man-made in origin, they can be natural. Examples include municipal and industrial discharges, combined sewer overflow, urban runoff, agricultural runoff, atmospheric deposition, rainfall, and subsurface runoff. Indirect boundary loads also can be originally man-made. These loads derive from upstream and downstream water concentrations, as well as benthic and atmospheric concentrations.

Transformation includes a diverse set of water quality kinetics and equilibria, which describe the important interactions among the water quality constituents. Transformations are independent of location per se, although they are functions of exogenous variables such as temperature, light, and pH, which may vary with location and time. The same transformation equations are used for each location throughout the water body. Thus, given local values of the exogenous variables, the rate or extent to which any transformation proceeds is controlled by the local constituent concentrations.

1.3.3 The Model Network

The model network is a set of expanded control volumes, or "segments," that together represent the physical configuration of the water body. As Figure 17 illustrates, the network may subdivide the water body laterally and vertically as well as longitudinally. Benthic segments can be included along with water column segments. If the water quality model is being linked to the hydrodynamic model, then water column segments must correspond to the hydrodynamic junctions. Concentrations of water quality constituents are calculated within each segment. Transport rates of water quality constituents are calculated across the interface of adjoining segments.

Segment volumes and the simulation time step are directly related. As one increases or decreases, the other must do the same to insure stability and numerical accuracy. Segment size can vary dramatically, as illustrated in Figure 18. Characteristic sizes are dictated primarily by the spatial and temporal scale of the problem being analyzed. This is more important than the characteristics of the water body or the pollutant per se. For example, analyzing a problem involving the upstream tidal migration of a pollutant into a water supply might require a time step of minutes to an hour. By contrast, analyzing a problem involving the total residence time of that

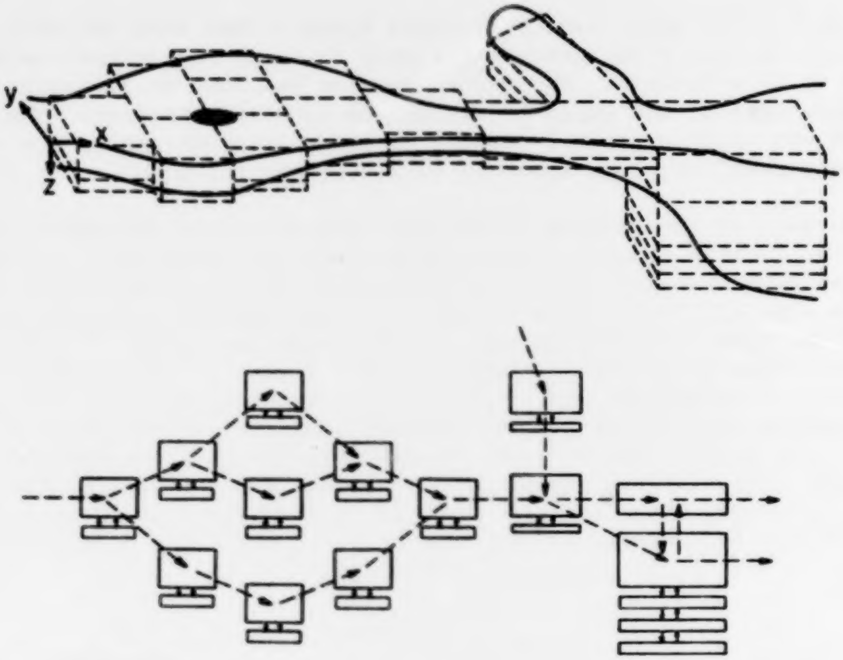


Figure 17. Model segmentation

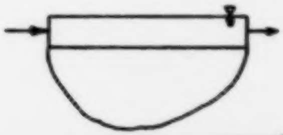
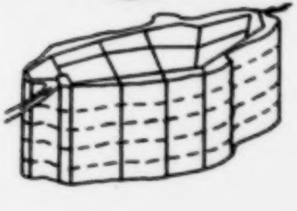
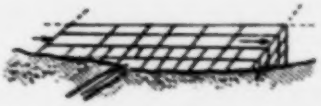
MODEL DESIGNATION		NUMBER OF SEGMENTS	HORIZONTAL SCALE (km²) EPILIMNION SEGMENTS
LAKE 1		2	13,000
LAKE 3		67	200-1000
ROCHESTER EMBAYMENT		72	10-100

Figure 18. Spatial scales used in Lake Ontario Analysis.

pollutant in the same water body could allow a time step of hours to a day. In Figure 18, the first network was used to study the general eutrophic status of Lake Ontario. The second network was used to investigate the lake-wide spatial and seasonal variations in eutrophication. The third network was used to predict changes in near-shore eutrophication of Rochester Embayment resulting from specific pollution control plans.

As part of the problem definition, the user must determine how much of the water quality frequency distribution must be predicted. For example, a daily-average dissolved oxygen concentration of 5 mg/L would not sufficiently protect fish if fluctuations result in concentrations less than 2 mg/L for 10% of the time. Predicting extreme concentration values is generally more difficult than predicting average values. Figure 19 illustrates typical frequency distributions predicted by three model time scales and a typical distribution observed by rather thorough sampling as they would be plotted on probability paper. The straight lines imply normal distributions. Reducing the model time step (and consequently segment size) allows better simulation of the frequency distribution. This increase in predictive ability, however, also entails an increase in the resolution of the input data.

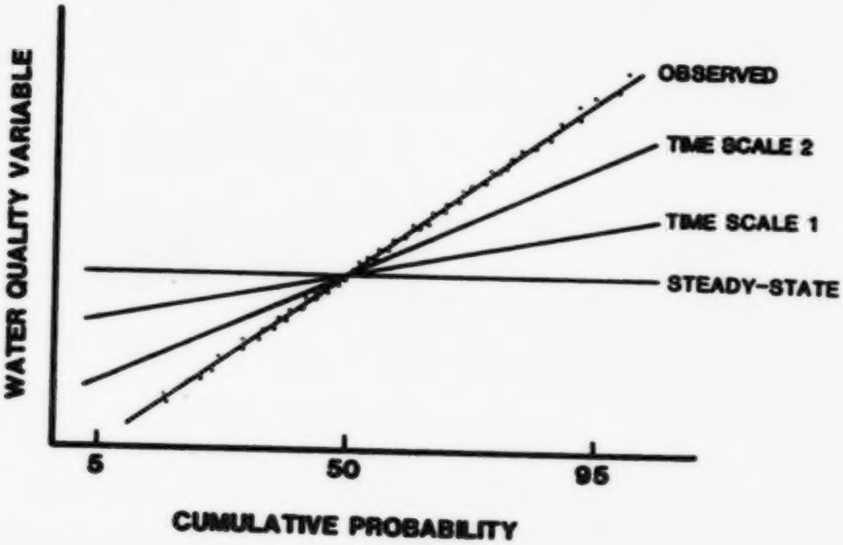


Figure 19. Frequency distribution of observed and calculated values of a quality variable.

Once the nature of the problem has been determined, then the temporal variability of the water body and input loadings must be considered. Generally, the model time step must be somewhat less than the period of variation of the important driving variables. In some cases, this restriction can be relaxed by averaging the input over its period of variation. For example, phytoplankton growth is driven by sunlight, which varies diurnally. Most eutrophication models, however, average the light input over a day, allowing time steps on the order of a day.

Care must be taken so that important non-linear interactions do not get averaged out. When two or more important driving variables have a similar period of variation, then averaging may not be possible. One example is the seasonal variability of light, temperature, nutrient input, and transport in lakes subject to eutrophication. Another example involves discontinuous batch discharges. Such an input into a large lake might safely be averaged over a day or week, because large scale transport variations are relatively infrequent. The same batch input into a tidal estuary cannot safely be averaged, however, because of the semi-diurnal or diurnal tidal variations. A third example is salinity intrusion in estuaries. Tidal variations in flow, volume, and dispersion can interact so that accurate long-term predictions require explicit simulation at time steps on the order of hours.

Once the temporal variability has been determined, then the spatial variability of the water body must be considered. Generally, the important spatial characteristics must be homogeneous within a segment. In some cases, this restriction can be relaxed by judicious averaging over width, depth, and/or length. For example, depth governs the impact of reaeration and sediment oxygen demand in a column of water. Nevertheless, averaging the depth across a river would generally be acceptable in a conventional waste load allocation, whereas averaging the depth across a lake would not generally be acceptable. Other important spatial characteristics to consider (depending upon the problem being analyzed) include temperature, light penetration, velocity, pH, benthic characteristics or fluxes, and sediment concentrations.

The expected spatial variability of the water quality concentrations also affects the segment sizes. The user must determine how much averaging of the concentration gradients is acceptable. Because water quality conditions change rapidly near a loading point and stabilize downstream, studying the effects on a beach a quarter-mile downstream of a discharge requires smaller segments than studying the effects on a beach several miles away.

A final, general guideline may be helpful in obtaining accurate simulations: water column volumes should be roughly the same. If flows vary significantly downstream, then segment volumes should increase proportionately. The user should first choose the proper segment volume and time step in the critical reaches of the water body (V_c, Δt_c), then scale upstream and downstream segments accordingly:

$$V_i = V_c \cdot Q_i/Q_c \qquad 31$$

Of course, actual volumes specified must be adjusted to best represent the actual spatial variability, as discussed above. This guideline will allow larger time steps and result in greater numerical accuracy over the entire model network, as explained in Section 1.3.5.6.

1.3.4 Implementation of the Mass Balance Equation

WASP solves a finite difference approximation of equation 29 for a model network that represents the important characteristics of the real water body. This section explains the derivation of WASP's finite difference mass balance equation using the one-dimensional form for convenience. Regrouping the terms in 30 for mathematical convenience gives:

$$\frac{\partial}{\partial t}(A \cdot C) = -\frac{\partial}{\partial x}(Q \cdot C) + \frac{\partial}{\partial x}\left(E_x \cdot A \cdot \frac{\partial C}{\partial x}\right) + A \cdot S^T \qquad 32$$

where:

S^T = total source/sink rate = $S_L + S_B + S_K$, ML^3/T

Q = volumetric flow = $A \cdot U_x$, L^3/T

Assuming that derivatives of C are single-valued, finite, continuous functions of x, as in Figure 20, then the Taylor's series expansion gives:

$$C_{x_o+\Delta x} = C_{x_o} + \Delta x \cdot \frac{\partial C}{\partial x}\bigg|_{x_o} + \frac{1}{2}\Delta x^2 \cdot \frac{\partial^2 C}{\partial x^2}\bigg|_{x_o} + \frac{1}{6}\Delta x^3 \cdot \frac{\partial^3 C}{\partial x^3}\bigg|_{x_o} + \ldots \qquad 33$$

$$C_{x_o-\Delta x} = C_{x_o} - \Delta x \cdot \frac{\partial C}{\partial x}\bigg|_{x_o} + \frac{1}{2}\Delta x^2 \cdot \frac{\partial^2 C}{\partial x^2}\bigg|_{x_o} - \frac{1}{6}\Delta x^3 \cdot \frac{\partial^3 C}{\partial x^3}\bigg|_{x_o} + \ldots \qquad 34$$

Assuming that terms containing the third and higher powers of Δx are negligible in comparison with the lower powers of Δx, then equations 33 and 34 can be subtracted to give:

$$\frac{\partial c}{\partial x}\bigg|_{x_o} = \frac{C_{x_o+\Delta x} - C_{x_o-\Delta x}}{2\Delta x} \qquad 35$$

with an error term of order Δx^2. Referring to Figure 20, this equation states that the slope of the line AB is equal to the slope of the tangent centered at P. This is known as the central-difference approximation. The slope at P may also be approximated by the slope of the line PB, giving the forward-difference formula:

$$\frac{\partial c}{\partial x}\bigg|_{x_o} = \frac{C_{x_o+\Delta x} - C_{x_o}}{\Delta x} \qquad 36$$

Similarly, the slope at P may be approximated by the slope of the line AP, giving the backward-difference formula:

$$\frac{\partial c}{\partial x}\bigg|_{x_o} = \frac{C_{x_o} - C_{x_o-\Delta x}}{\Delta x} \qquad 37$$

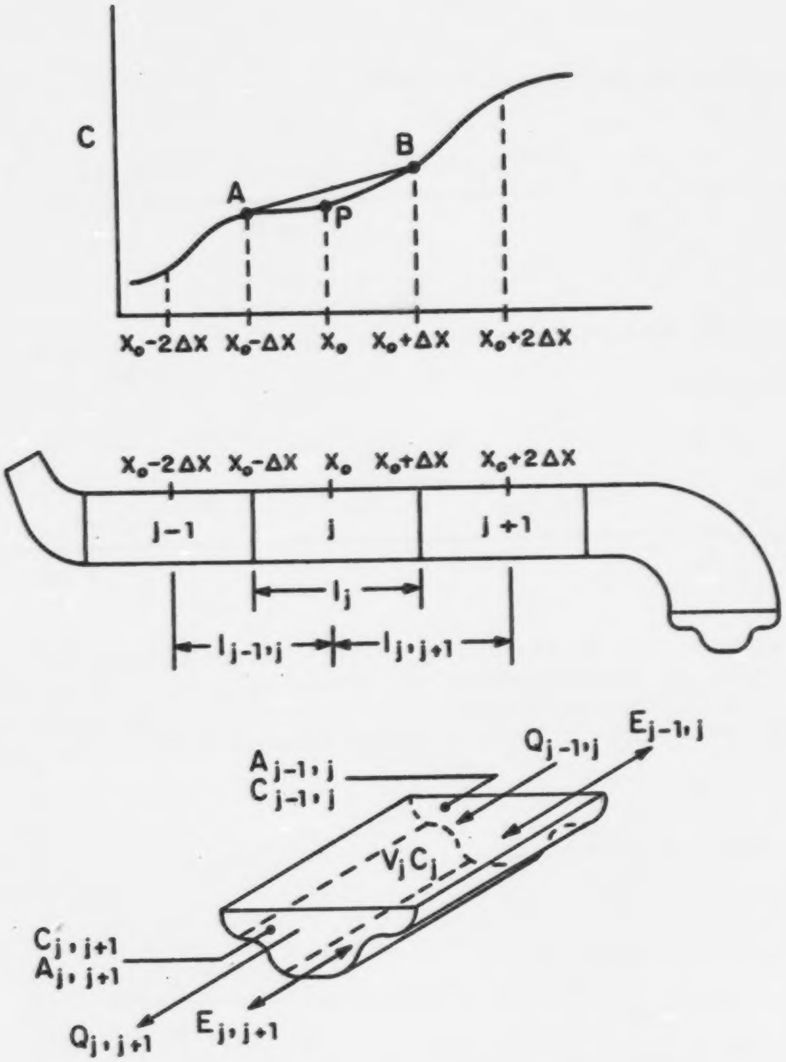

C
A
P
B
$X_o-2\Delta X$
$X_o-\Delta X$
X_o
$X_o+\Delta X$
$X_o+2\Delta X$
$X_o-2\Delta X$
$X_o-\Delta X$
X_o
$X_o+\Delta X$
$X_o+2\Delta X$
j−1
j
j+1
l_j
$l_{j-1,j}$
$l_{j,j+1}$
$A_{j-1,j}$
$C_{j-1,j}$
$Q_{j-1,j}$
$E_{j-1,j}$
V_jC_j
$C_{j,j+1}$
$A_{j,j+1}$
$Q_{j,j+1}$
$E_{j,j+1}$

Figure 20. Definition sketch for finite difference equation.

Equations 36 and 37 can be obtained from 33 and 34, respectively, by assuming the second and higher order powers of Δx are negligible. The error term for both the forward-difference and the backward difference approximation is of order Δx.

Substituting the central difference approximation into the advection term of 32 gives:

$$\frac{\partial}{\partial x}(Q.C) = \frac{Q_{x_o+\Delta x} \,.\, C_{x_o+\Delta x} - Q_{x_o-\Delta x} \,.\, C_{x_o-\Delta x}}{2\,\Delta x} \tag{38}$$

Similarly, the dispersion term becomes:

$$\frac{\partial}{\partial x}\left(E_x \,.\, A \,.\, \frac{\partial c}{\partial x}\right) = \frac{(E.A)_{x_o+\Delta x} \,.\, \left.\frac{\partial c}{\partial x}\right|_{x_o+\Delta x} - (E.A)_{x_o-\Delta x} \,.\, \left.\frac{\partial c}{x}\right|_{x_o-\Delta x}}{2\,\Delta x} \tag{39}$$

Substituting the central difference approximation into $\left.\frac{\partial c}{\partial x}\right|_{x_o+\Delta x}$ in equation 39 gives:

$$\frac{\partial}{\partial x}\left(E_x.A.\frac{\partial c}{\partial x}\right) = \frac{(E.A)_{x_o+\Delta x} \,.\, \dfrac{C_{x_o+2\Delta x} - C_{x_o}}{2\Delta x}}{2\,\Delta x} - \frac{(E.A)_{x_o-\Delta x} \dfrac{C_{x_o} - C_{x_o-2\Delta x}}{2\,\Delta x}}{2\,\Delta x} \tag{40}$$

When applying the difference approximations to segment "j" in a network as in Figure 20, x_o corresponds to the center of j, $x_o + \Delta x$ to the interface j, j+1, $x_o - \Delta x$ to the interface j-1, j, $x_o + 2\,\Delta x$ to the center of j+1, and $x_o - 2\,\Delta x$ to the center of j-1. The mass balance equation for segment j can be written:

$$\begin{aligned}\frac{\partial}{\partial t}(A_j.C_j) = {} & -\frac{Q_{j,j+1}}{\ell_j} \,.\, C_{j,j+1} + \frac{Q_{j-1,j}}{\ell_j} \,.\, C_{j-1,j} \\ & + \frac{(E.A)_{j,j+1}}{\ell_j \,.\, \ell_{j,j+1}} \,.\, (C_{j+1} - C_j) - \frac{(E.A)_{j-1,j}}{\ell_j \,.\, \ell_{j-1,j}} \,.\, (C_j - C_{j-1}) \\ & + A_j \,.\, S_j^T \end{aligned} \tag{41}$$

Multiplying through by ℓ_j gives:

$$\begin{aligned}\frac{\partial}{\partial t}(V_j \,.\, C_j) = {} & - Q_{j,j+1} \,.\, C_{j,j+1} + Q_{j-1} \,.\, C_{j-1,j} \\ & + R_{j,j+1} \,.\, (C_{j+1} - C_j) - R_{j-1,j} \,.\, (C_j - C_{j-1}) \\ & + V_j \,.\, S_j^T \end{aligned} \tag{42}$$

where:

V_j = volume of segment j = $A_j \cdot \ell_j$, L^3

R = dispersive flow = $\frac{E.A}{\ell}$, L^3/T

ℓ = characteristic length, L

Interface concentrations $C_{j,j+1}$ and $C_{j-1,j}$ must be expressed in terms of the segment concentrations:

$$C_{j,j+1} = \nu \cdot C_{j+1} + (1 - \nu) \cdot C_j \quad 43$$

$$C_{j-1,j} = \nu \cdot C_j + (1 - \nu) \cdot C_{j-1} \quad 44$$

where:

ν = numerical weighting factor between 0 and 1

Specifying $\nu = 0$ gives a backward difference approximation for the advective term, whereas $\nu = \frac{1}{2}$ gives a central difference approximation.

Equation 42 can be extended to the multi-dimensional form actually employed by WASP. Consider "i" segments adjoining segment j. Interfaces are denoted "ij." The general equation becomes:

$$\frac{\partial}{\partial t}(V_j \cdot C_j) = -\sum_i Q_{ij} \cdot C_{ij} + \sum_i R_{ij} \cdot (C_i - C_j) + W_j + \sum_B V_j \cdot S_{B_j} + \sum_k V_j \cdot S_{K_j} \quad 45$$

where:

Q_{ij} = flow, defined as positive when leaving segment j, and negative when entering j, L^3/T

W_j = point and diffuse loads = $V_j S_{Lj}$, M/T

Equation 45 is the general expression used in WASP to evaluate the mass derivatives for every segment "j" during each time step "t" between initial time t_o and final time t_F. Given concentrations and volumes at t, WASP3 calculates new masses at t+Δt using the one-step Euler scheme:

$$(V_j \cdot C_j)_{t+\Delta t} = (V_j \cdot C_j)_t + \frac{\partial}{\partial t}(V_j \cdot C_j)_t \cdot \Delta t \quad 46$$

where:

Δt = the time step, typically between 15 minutes and a half day, T

Given new masses at time t + Δt, WASP3 finds the new concentrations by dividing by the new volumes:

$$C_{j,t+\Delta t} = (V_j \cdot C_j)_{t+\Delta t} / V_{j,t+\Delta t} \qquad 47$$

The new volumes are calculated internally from the specified (or computed) flow fields using the principle of continuity.

During normal simulations, WASP prohibits segment concentrations from going negative and causing numerical instability of the solution. A negative concentration might be calculated for constituents with low concentrations in the vicinity of significant spatial gradients. If a calculated mass derivative would drive a segment concentration below zero at t+Δt, WASP maintains a positive segment concentration by halving the mass present at time t. Experience has shown that this procedure is generally acceptable. The user can avoid this correction by specifying the proper value for the negative solution option. If negative concentrations and instability then occur, the simulation can be rerun with a smaller time step.

1.3.5 The Model Parameters

This section summarizes the input parameters that must be specified in order to solve the mass balance equation.

1.3.5.1 Model Identification Parameters

These parameters give the basic model identity. They include the number of water quality constituents being simulated and the number of segments in the network. Also included are user-specified simulation identification numbers and titles describing the water body and the simulation.

1.3.5.2 Transport Parameters

This broad group of parameters describes the network of segments representing the water body along with the advective and dispersive flow fields connecting the segments. Input parameters include segment volumes, advective flows, dispersion coefficients, cross-sectional areas, and characteristic lengths. While the nominal units expected by the model are English (ft, miles, etc.), SI or other units can be used along with proper specification of conversion factors.

Segment volume, million ft^3--Initial volumes for each segment can be calculated from navigation charts or a series of transects measuring depth versus width along the river. Sometimes, volumes can be estimated from travel time of a well-mixed cloud of dye through a reach. Initial segment volumes can be automatically adjusted for continuity during a simulation by specifying IVOPT = 2. For simulations using hydrodynamic results from DYNHYD3, volumes from the SUMRY2 file are used and continuity is maintained.

Advective flow, ft^3/sec--Steady or unsteady flows can be specified between adjoining segments, as well as entering or leaving segments as inflow or outflow. The user must be careful to check for continuity errors, as the model does not necessarily require that flow continuity be maintained. For example, the user may specify that more flow enters a segment than leaves. If IVOPT = 2, continuity will be maintained and that segment will grow in volume indefinitely. If IVOPT = 1, however, the volume will remain constant and pollutant mass will build up in the segment indefinitely. This corresponds to the case of a significant evaporative loss, which is not modeled explicitly. For simulations using hydrodynamic results from DYNHYD3, flows from the SUMRY2 file are used and flow continuity is automatically maintained.

Dispersion coefficient, mi^2/day--Dispersive mixing coefficients can be specified between adjoining segments, or across open water boundaries. The nominal input units were traditional for estuary studies in the United States. These coefficients can model pore water diffusion in benthic segments, vertical diffusion in lakes, and lateral and longitudinal dispersion in large water bodies. Values can range from 10^{-6} cm^2/sec for molecular diffusion to $5x10^6$ cm^2/sec for longitudinal mixing in some estuaries (3.33×10^{-12} to 16.7 square miles per day).

Cross-sectional area, ft^2--Cross-sectional areas are specified for each dispersion coefficient, reflecting the area through which mixing occurs. These can be surface areas for vertical exchange, such as in lakes or in the benthos. Areas are not modified during the simulation to reflect flow changes.

Characteristic mixing length, ft--Mixing lengths are specified for each dispersion coefficient, reflecting the characteristic length over which mixing occurs. These are typically the lengths between the center points of adjoining segments. A single segment may have three or more mixing lengths for segments adjoining longitudinally, laterally, and vertically. For surficial benthic segments connecting water column segments, the depth of the benthic layer is a more realistic mixing length than half the water depth.

1.3.5.3 Boundary Parameters

This group of parameters includes boundary concentrations and waste loads.

Boundary concentration, mg/L--Steady or time-variable concentrations must be specified for each water quality constituent at each boundary. A boundary is either a tributary inflow, a downstream outflow, or an open water end of the model network across which dispersive mixing can occur. Advective and dispersive flows across boundaries are specified by the transport parameters.

Waste load, lb/day--Steady or time-variable loads may be specified for each water quality constituent at several segments. These loads represent municipal and industrial wastewater discharges, urban and agricultural runoff, precipitation, and atmospheric deposition of pollutants.

1.3.5.4 Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated. None are necessary for dissolved, conservative chemicals.

1.3.5.5 Initial Conditions

This category includes only initial concentrations.

Initial concentration, mg/L--Concentrations of each constituent in each segment must be specified for the time at which the simulation begins. For those water bodies with low transport rates, the initial concentrations of conservative substances may persist for a long period of time. Accurate simulation, then, would require accurate specification of initial concentrations. If initial concentrations cannot be determined accurately, then longer simulations should be run, and early predictions discounted.

1.3.5.6 Simulation Parameters

This group of parameters controls the simulation and checks the stability of the solution. Simulation parameters include the initial and final times, integration time steps, the advection factor, maximum and minimum concentrations, and a negative solution option.

Initial time, days--The time at the beginning of the simulation must be specified in order to synchronize all the time functions. The day, hour, and minute can be input, or the day (including decimal fraction).

Final time, days--The time at the end of the simulation must be specified in days (including decimal fraction).

Integration time step, days--A sequence of integration time steps (Δt) must be specified, along with the time interval over which they apply. Given specific network and transport parameters, time steps are constrained within a specific range to maintain stability and minimize numerical dispersion, or solution inaccuracies. To maintain stability at a segment, the advected, dispersed, and transformed mass must be less than the resident mass:

$$(\sum Q \cdot C_j + \sum R \cdot C_j + \sum S \cdot V_j) \cdot \Delta t < V_j \cdot C_j \qquad 48$$

Solving for Δt and applying the criterion over the entire network gives the maximum stable step size:

$$\Delta t_{max} = \text{Min} \left(\frac{V_j}{\sum_i Q_{ij} + \sum_i R_{ij} + \sum_k S_{jk} \cdot V_j/C_j} \right) \qquad 49$$

If reactions are linear, then the last term in the denominator reduces to $K_j^T \cdot V_j$. Usually Δt is controlled by advective or dispersive flows.

Numerical dispersion is artificial mixing caused by the finite difference approximation used for the derivatives. If the advection factor $\nu = 0$, the backward difference approximation of $\partial c/\partial x$ is used in the advection term, and

$$E_{num} = \frac{U \cdot \ell}{2} \qquad 50$$

where:

ℓ = length of the segment

For the Euler scheme, the forward difference approximation of $\partial c/\partial t$ is used, and

$$E_{num} = -\frac{U^2 \cdot \Delta t}{2} \qquad 51$$

The total numerical dispersion, then, is

$$E_{num} = \frac{U}{2} \cdot (\ell - U \cdot \Delta t) \qquad 52$$

Note that increasing the time step up to $\Delta x/U$ (or V/Q) decreases numerical dispersion to 0. The conditions for stability discussed above require a time step somewhat less than V/Q for most segments. So to maintain stability and minimize numerical dispersion in a water body subject to unsteady flow, the sequence of time steps must be as large as possible, but always less than Δt_{max} given in 49.

Advection factor, dimensionless--The advection factor ν can be specified to modify the finite difference approximation of $\partial c/\partial x$ used in the advection term by WASP. For $\nu = 0$, the backward difference approximation is used. This is most stable, and is recommended for most applications. For $\nu = 0.5$, the central difference approximation is used. This is unstable in WASP, and is not recommended.

A nonzero advection factor is helpful in situations where the network size and time step produce large numerical dispersion. A nonzero advection factor reduces the numerical dispersion produced by a particular velocity, length, and time step combination. According to Bella and Grenney (1970):

$$E_{num} = \frac{U}{2} \cdot [(1-2 \cdot \nu) \cdot \ell - U \cdot \Delta t] \qquad 53$$

Note that a ν of 0 reduces this to equation 52. Values of E_{num} for a length of 2000 meters and various combinations of velocity and time step are provided in Table 2. For a particular velocity, say 0.4 m/sec, numerical dispersion can be reduced by increasing the time step. For $\nu = 0$, increasing the time step from 1000 to 4000 seconds decreases E_{num} from 320 to 80 m^2/sec. If the time step must be 1000 seconds, however, numerical dispersion can still be reduced by increasing ν. In this case, increasing ν from 0 to 0.4 decreases E_{num} from 320 to 0 m^2/sec.

Maximum and minimum concentrations, mg/L--Maximum and minimum concentrations must be specified for each water quality constituent. The simulation is automatically aborted if a calculated concentration falls outside these limits. This usually indicates computational instability, and the time step must usually be reduced. Minimum concentrations are usually set to 0, and maximum concentrations to physically unrealistic values.

Negative solution option--Normally, concentrations are not allowed to become negative. If a predicted concentration at t+ Δt is negative, WASP maintains its positive value by instead halving the concentration at time t. The negative solution option lets the user bypass this procedure, allowing negative concentrations. This may be desirable for simulating dissolved oxygen deficit in the benthos, for example.

1.3.6 Application of the Model

The first step in applying the model is analyzing the problem to be solved. What questions are being asked? How can a simulation model be used to address these questions? A water quality model can do three basic tasks--describe present water quality conditions, provide generic predictions, and provide site-specific predictions. The first, descriptive task is to extend in some way a limited site-specific data base. Because monitoring is expensive, data seldom give the spatial and temporal resolution needed to fully characterize a water body. A simulation model can be used to interpolate between observed data, locating, for example, the dissolved oxygen sag point in a river or the maximum salinity intrusion in an estuary. Of course such a model can be used to guide future monitoring efforts. Descriptive models also can be used to infer the important processes controlling present water quality. This information can be used to guide not only monitoring efforts, but also model development efforts.

Providing generic predictions is a second type of modeling task. Site-specific data may not be needed if the goal is to predict the types of water bodies at risk from a new chemical. A crude set of data may be adequate to screen a list of chemicals for potential risk to a particular water body. Generic predictions may sufficiently address the management problem to be solved, or they may be a preliminary step in detailed site-specific analyses.

TABLE 2. VALUES OF NUMERICAL DISPERSION IN m^2/sec

	U (m/sec)					
ν	0.1	0.2	0.4	0.6	0.8	1.0
	Δt = 1000 sec					
0.0	95	180	320	420	480	500
0.1	75	140	240	300	320	300
0.2	55	100	160	180	160	100
0.3	35	60	80	60	0	--
0.4	15	20	0	--	--	--
	Δt = 2000 sec					
0.0	90	160	240	240	160	0
0.1	70	120	160	120	0	--
0.2	50	80	80	0	--	--
0.3	30	40	0	--	--	--
0.4	10	0	--	--	--	--
	Δt = 4000 sec					
0.0	80	120	80	--	--	--
0.1	60	80	0	--	--	--
0.2	40	40	--	--	--	--
0.3	20	0	--	--	--	--
0.4	0	--	--	--	--	--
	Δt = 8000 sec					
0.0	60	40	--	--	--	--
0.1	40	0	--	--	--	--
0.2	20	--	--	--	--	--
0.3	0	--	--	--	--	--
0.4	--	--	--	--	--	--

Providing site-specific predictions is the most stringent modeling task. Calibration to a good set of monitoring data is definitely needed to provide credible predictions. Because predictions often attempt to extrapolate beyond the present data base, however, the model also must have sufficient process integrity. Examples of this type of application include waste load allocation to protect water quality standards and feasibility analysis for remedial actions, such as tertiary treatment, phosphate bans, or agricultural best-management practices.

Analysis of the problem should dictate the spatial and temporal scales for the modeling analysis. Division of the water body into appropriately sized segments was discussed in Section 1.3.3. The user must try to extend the network upstream and downstream beyond the influence of the waste loads being studied. If this is not possible, the user should extend the network far enough so that errors in specifying future boundary concentrations do not propogate into the reaches being studied.

The user also should consider aligning the network so that sampling stations and points of interest (such as water withdrawals) fall near the center of a segment. Point source waste loads in streams and rivers with unidirectional flow should be located near the upper end of a segment. In estuaries and other water bodies with oscillating flow, waste loads are best centered within segments. If flows are to be input from DYNHYD3, then a WASP3 segment must coincide with each hydrodynamic junction. Benthic segments, which are not present in the hydrodynamic network, may nevertheless be included in the WASP3 network. Furthermore, WASP segment numbering does not have to be the same as DYNHYD3 junction numbering. General segment numbering is arbitrary, except in TOXIWASP, where segments stacked vertically must be numbered consecutively from surface water down.

Once the network is set up, the model study will proceed through four general steps involving, in some manner, hydrodynamics, mass transport, water quality transformations, and environmental toxicology. The first step addresses the question of where the water goes. This can be answered by a combination of gaging, special studies, and hydrodynamic modeling. Flow data can be interpolated or extrapolated using the principle of continuity. Very simple flow routing models can be used; very complicated multi-dimensional hydrodynamic models can also be used with proper averaging over time and space. At present, the most compatible hydrodynamic model is DYNHYD3.

The third step answers the question of how the material in the water and sediment is transformed and what is its fate. This is the main focus of many studies. Answers depend on a combination of laboratory studies, field monitoring, parameter estimation, calibration, and testing. The net result is sometimes called model validation or verification, which are elusive concepts. The success of this step depends on the skill of the user, who must combine specialized knowledge with common sense and skepticism into a methodical process.

The final step answers the question of how this material is likely to affect anything of interest, such as people, fish, or the ecological balance.

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Often, predicted concentrations are simply compared with water quality criteria adopted to protect the general aquatic community. Care must be taken to insure that the temporal and spatial scales assumed in developing the criteria are compatible with those predicted by the model. Sometimes principles of physical chemistry or pharmacokinetics are used to predict chemical body burdens and resulting biological effects. This field holds promise, but is still in its infancy.

1.4 THE EUTROPHICATION MODEL

The eutrophication model, EUTRWASP, is a simplified version of the Potomac Eutrophication Model, PEM (Thomann and Fitzpatrick, 1982). The following text is taken from the PEM documentation report, with little modification.

1.4.1 Overview of EUTRWASP

Several physical-chemical processes can affect the transport and interaction among the nutrients, phytoplankton, carbonaceous material, and dissolved oxygen in the aquatic environment. Figure 21 presents the principal kinetic interactions for the nutrient cycles and dissolved oxygen. Consider phosphorus: dissolved or available phosphorus is utilized by phytoplankton for growth and interacts with particulate inorganic phosphorus via a sorption-desorption mechanism. Phosphorus is returned from the phytoplankton biomass pool to dissolved and particulate organic phosphorus and to dissolved inorganic phosphorus through endogenous respiration and non-predatory mortality. Organic phosphorus is converted to dissolved inorganic phosphorus at a temperature-dependent rate.

The kinetics of the nitrogen species are fundamentally the same as the phosphorus system. Ammonia and nitrate are used by phytoplankton for growth. The rate at which each is taken up is proportional to its concentration relative to the total inorganic nitrogen (ammonia plus nitrate) available. Nitrogen is returned from the algal biomass and follows pathways that are similar to phosphorus. Organic nitrogen is converted to ammonia at a temperature dependent rate, and ammonia is then converted to nitrate (nitrification) at a temperature- and oxygen-dependent rate. Nitrate may be converted to nitrogen gas (denitrification) in the absence of oxygen and at a temperature-dependent rate.

Dissolved oxygen is coupled to the other state variables. The sources of oxygen considered are reaeration, evolution by phytoplankton during growth, and evolution during denitrification. The sinks of oxygen are algal respiration, oxidation of detrital carbon and carbonaceous material from waste effluents and nonpoint discharges, and nitrification.

EUTRWASP simulates the transport and transformation reactions of eight state variables, illustrated in Figure 22. They can be considered as four interacting systems: phytoplankton kinetics, the phosphorus cycle, the

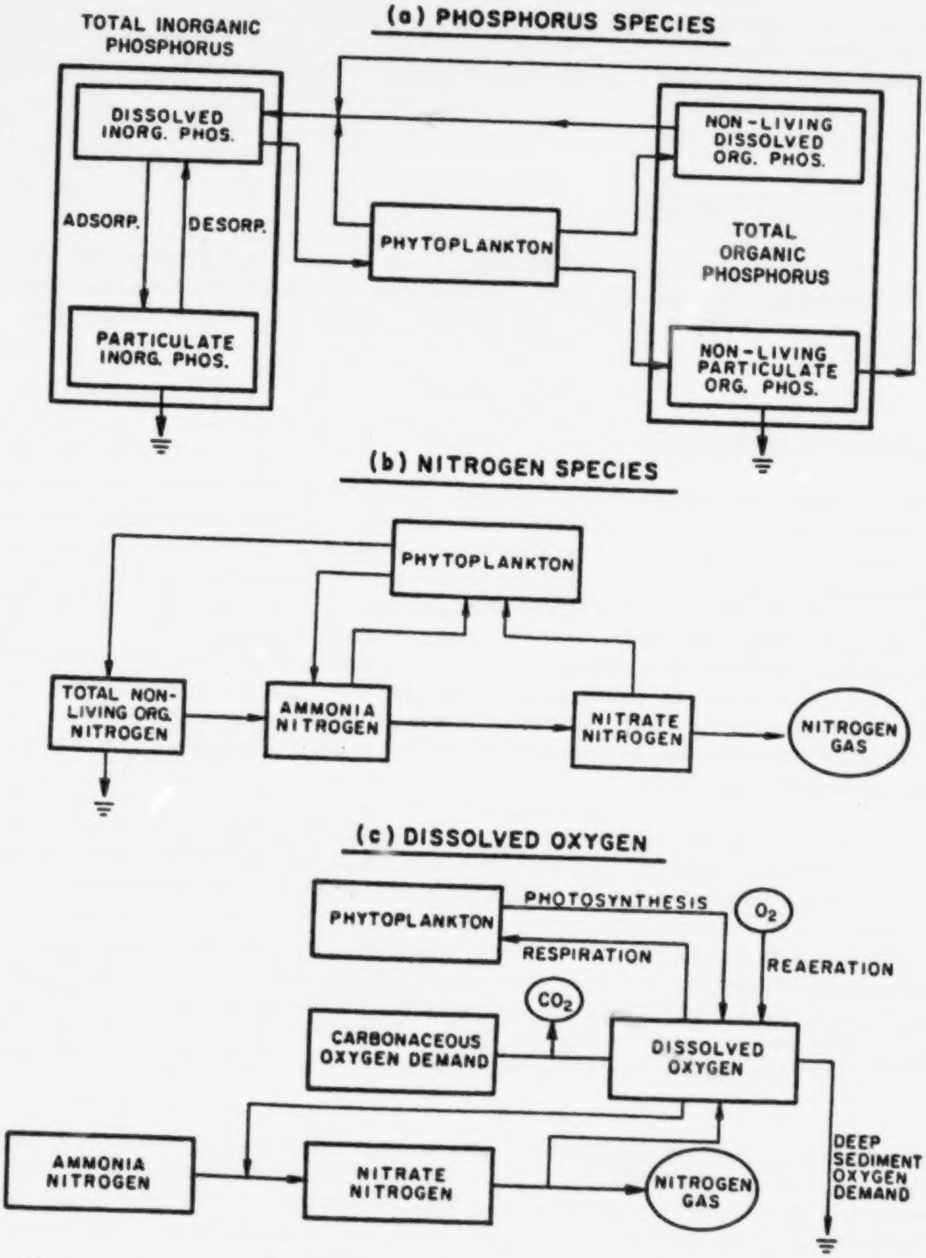
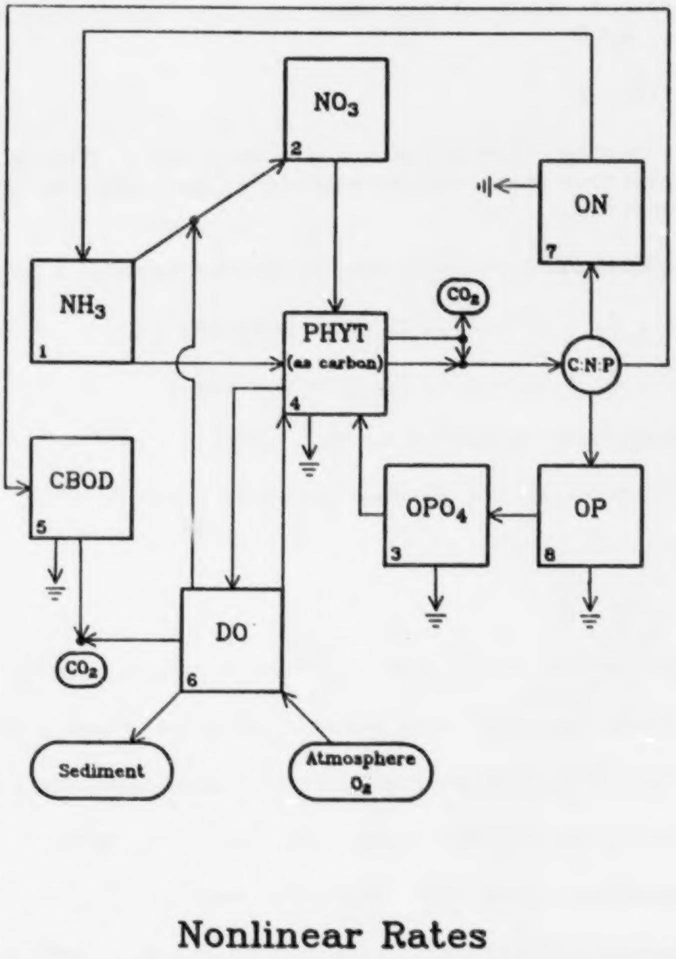

(a) PHOSPHORUS SPECIES
TOTAL INORGANIC PHOSPHORUS
DISSOLVED INORG. PHOS.
ADSORP.
DESORP.
PARTICULATE INORG. PHOS.
PHYTOPLANKTON
NON-LIVING DISSOLVED ORG. PHOS.
TOTAL ORGANIC PHOSPHORUS
NON-LIVING PARTICULATE ORG. PHOS.
(b) NITROGEN SPECIES
PHYTOPLANKTON
TOTAL NON-LIVING ORG. NITROGEN
AMMONIA NITROGEN
NITRATE NITROGEN
NITROGEN GAS
(c) DISSOLVED OXYGEN
PHYTOPLANKTON
PHOTOSYNTHESIS
RESPIRATION
O_2
REAERATION
CO_2
CARBONACEOUS OXYGEN DEMAND
DISSOLVED OXYGEN
AMMONIA NITROGEN
NITRATE NITROGEN
NITROGEN GAS
DEEP SEDIMENT OXYGEN DEMAND

Figure 21. EUTRWASP state variable interactions.



NO_3
2
ON
7
NH_3
1
CO_2
PHYT
(as carbon)
4
C:N:P
CBOD
5
OPO_4
3
OP
8
DO
6
CO_2
Sediment
Atmosphere
O_2
Nonlinear Rates

Figure 22. EUTRWASP state variable interactions.

nitrogen cycles and the dissolved oxygen balance. The general WASP3 mass balance equation is solved for each state variable:

$$\frac{\Delta\ (V_j \cdot C_j)}{\Delta t} = \sum_i \left[-Q_{ij} \cdot C_{ij} + R_{ij} \cdot (C_i - C_j)\right]$$

$$+ \sum_L W_{Lj} + \sum_B W_{Bj} + \sum_k V_j \cdot S_{kj} \qquad 54$$

where:

C_j = concentration of the water quality constituent in segment j, M/L^3

t = time, T

Q_{ij} = advective flow between segments i and j, defined as positive when leaving segment j, and negative when entering, L^3/T

C_{ij} = constituent concentration advected between i and j, ML^{-3}

= $\nu \cdot C_j + (1 - \nu) \cdot C_i$ when entering j

= $\nu \cdot C_i + (1 - \nu) \cdot C_j$ when leaving j

ν = numerical weighting factor, 0-0.5

R_{ij} = dispersive flow between segments i and j, L^3/T

$$= \frac{E_{ij} \cdot A_{ij}}{\ell_{ij}}$$

E_{ij} = dispersion coefficient between segments i and j, L^2/T

A_{ij} = cross-sectional area between segments i and j, L^2

ℓ_{ij} = characteristic mixing length between segments i and j, L

W_{Lj} = point and diffuse loads into segment j, M/T

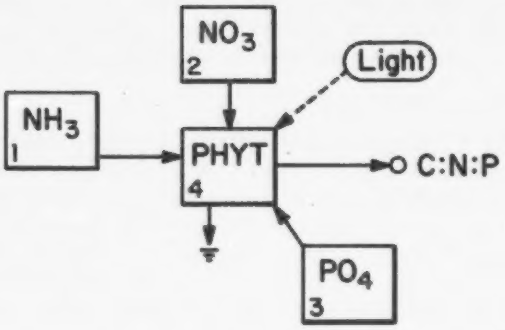
W_{Bj} = boundary loads into segment j, M/T

S_{kj} = kinetic transformations within segment j, $M/L^3/T$

To this general equation, the EUTRWASP subroutines add specific transport processes, including settling, deposition, scour, sedimentation, and benthic-water column dispersive exchange. The net effect is to customize equation 54 for the eight state variables in the water column and benthos. The rest of Section 1.4 covers the specific details for the several transformation sources and sinks S_{kj}.

1.4.2 Phytoplankton Kinetics

Phytoplankton kinetics assume a central role in eutrophication, affecting all other systems. An overview of this system is given in Figure 23.



C_4: Phytoplankton Carbon

$$\frac{\partial C_4}{\partial t} = \left(\underset{\text{growth}}{GPI} - \underset{\text{death}}{DPI} - \underset{\text{settling}}{\frac{SVPI}{d}}\right) \cdot C_4$$

Figure 23. Phytoplankton kinetics.

It is convenient to express the reaction term of phytoplankton, S_{1j}, as a difference between the growth rate, G_{1j}, of phytoplankton and their death rate, D_{1j}, in the volume V_j. That is:

$$S_{1j} = (G_{1j} - D_{1j}).P_j \qquad 55$$

where:

S_{1j} = reaction term, cells/ℓ.day

P_j = phytoplankton population, cells/ℓ

G_{1j} = growth rate, day^{-1}

D_{1j} = death rate, day^{-1}

j = segment number, unitless

The subscript 1 identifies the quantities as referring to phytoplankton type 1, (only one type is considered in this particular model); the subscript j refers to the volume element being considered. The balance between the magnitude of the growth rate and death rate (together with the transport and mixing) determines the rate at which phytoplankton mass is created in the volume element V_j.

As pointed out by Di Toro and Matystik (1980), the growth rate of a population of phytoplankton in a natural environment is a complicated function of the species of phytoplankton present and their differing reactions to solar radiation, temperature, and the balance between nutrient availability and phytoplankton requirements. The complex and often conflicting data pertinent to this problem have been reviewed by several researchers (Rhee ,1973; Hutchinson, 1967; Strickland, 1965; Lund, 1965; and Raymont, 1963). The available information is not sufficiently detailed to specify the growth kinetics for individual algal species in a natural environment. Hence, in order to accomplish the task of constructing a growth function, a simplified approach is followed. Rather than considering the problem of different species and their associated environmental and nutrient requirements, this model characterizes the population as a whole by the total biomass of the phytoplankton present.

For single species, the direct measure of the population size is the number of cells per unit of volume. For studies of a single species in a well-controlled laboratory environment these cell counts may be obtained fairly readily. In naturally occurring populations, however, this measure may be somewhat ambiguous: it is difficult to discern viable and non-viable cells, and species that tend to colonize pose a problem because the count usually does not distinguish individual cells and because the sizes of the colonies are quite variable.

The sum of the numbers of each species, the total count, is a possibility but because cell size varies substantially the nanoplankton would dominate such an aggregation. To account for this, the total bio-volume or wet weight of phytoplankton, assuming unit density, can be calculated using characteristic volumes for each identified species. Unfortunately, volumes can vary appreciably as a function of nutrient status. Conversion to phytoplankton dry weight and carbon involves further species-dependent constants that are also nutrient dependent and, therefore, are subject to variation and uncertainty. Thus, although the use of phytoplankton dry weight or carbon concentration is an appealing solution to the issue of aggregation, it suffers from some practical difficulties.

An alternate solution is to measure a parameter that is characteristic of all phytoplankton, namely, chlorophyll-a, and to use this as the aggregated variable. The principal advantages are that the measurement is direct; it integrates cell types and ages, and it accounts for cell viability. The principal disadvantage is that it is a community measurement with no differentiation of functional groups (e.g., diatoms, blue-greens); also, it is not necessarily a good measurement of standing crop in dry weight or carbon units because the chlorophyll-to-dry-weight and carbon ratios are variable and non-active chlorophyll (phaeopigments) must be measured to determine viable chlorophyll concentrations.

As can be seen from the above discussion, no simple aggregate measurement is entirely satisfactory. From a practical point of view, the availability of extensive chlorophyll data essentially dictates its use as the aggregate measure of the phytoplankton population or biomass for calibration and verification purposes. For internal computational purposes, however, EUTRO3 uses phytoplankton carbon as a measure of algal biomass. The reason for choosing phytoplankton carbon as the internal state variable reflects the decision to include a mechanism in the modeling framework that attempts to recognize the variable carbon to chlorophyll stoichiometry that occurs in the water body for a given temperature and light condition. If one had decided to use a fixed carbon-to-chlorophyll ratio and to use chlorophyll-a as a biomass measure it would be relatively simple to determine the equivalent algal carbon deposited in the sediment due to settling and to determine its equivalent sediment oxygen demand (SOD). The same could not be done if chlorophyll-a were still to be used as a biomass measure and if the carbon-to-chlorophyll ratio in the overlying water column was permitted to vary. One would not be able to determine the equivalent detrital carbon content of the sediment (and therefore the equivalent SOD) because the variable carbon-to-chlorophyll ratio determined for the overlying water column would not be valid for the sediment layer. Instead a dual approach is taken: (1) as stated previously, phytoplankton carbon is used as the internal state variable, which facilitates the computation of the sediment carbon and sediment oxygen demand; (2) using the variable carbon to chlorophyll mechanism (discussed subsequently), phytoplankton chlorophyll-a may be computed and used as the calibration and verification variable to be compared against observed chlorophyll-a field data.

With a choice of biomass units established, a growth rate that expresses the rate of production of biomass as a function of the important environmental variables (temperature, light, and nutrients) may be developed. The specific growth rate, G_{1j}, in segment j is related to G_{1max}, the maximum growth rate at optimum light, temperature, and nutrients, via the following equation.

$$G_{1j} = \underbrace{G_{1max}(T)}_{\text{temperature}} \cdot \underbrace{G(I)}_{\text{light}} \cdot \underbrace{G(N)}_{\text{nutrients}} \qquad 56$$

where:

$G(I)$ = the light attenuation as a function of I, f, H, and K_e:

$$G(I) = g(I, f, H, K_e) \qquad 57$$

$G(N)$ = the nutrient limitation as a function of DIP and DIN:

$$G(N) = g(DIP, DIN) \qquad 58$$

where:

T = ambient water temperature, °C

I = incident solar radiation, Ly/day

f = fraction of daylight, unitless

H = depth of the water column, ft

K_e = extinction or light attenuation coefficient, ft^{-1}

DIP,DIN = available nutrients for growth, dissolved inorganic phosphorus (orthophosphate) and dissolved inorganic nitrogen (ammonia plus nitrate), mg/l

An initial estimate of G_{1max} can be made based upon previous studies of phytoplankton dynamics and upon reported literature values (such as Zison et al., 1978) and subsequently refined during the calibration and verification process. The selected maximum growth rate must then be temperature-corrected using temporally- and spatially-variable water column temperatures as reported in field studies. The temperature-corrected growth rate is computed using:

$$G_{1max}(T) = G_{1max}(20°C) \cdot \theta_1^{(T-20)} \qquad 59$$

where:

θ_1 = temperature coefficient, unitless

Di Toro and Matystik (1980) report a value of 1.068 for θ_1. This temperature-corrected growth rate is then adjusted to reflect attenuation due to ambient light and nutrient levels.

In the natural environment, the light intensity to which the phytoplankton are exposed is not uniformly at the optimum value. At the surface and near-surface of the air-water interface, photoinhibition can occur at high light intensities, whereas at depths below the euphotic zone light is not available for photosynthesis due to natural and algal-related turbidity. A modeling framework developed by Smith (1980), extending upon a light curve analysis formulated by Steele (1962), accounts for both the effects of supersaturating light intensities and light attenuation through the water column. The depth-averaged growth rate developed by Smith is presented in Equation 60 and is obtained by integrating the specific growth rate over depth:

$$G(I) = G_{1max}(T) \cdot \frac{e}{K_e . H} \left[\exp\left(-\frac{I_o}{I_s} e^{-K_e . H}\right) - \exp\left(-\frac{I_o}{I_s}\right)\right] \qquad (60)$$

where:

$$I_s = \frac{G_{1max} \cdot \theta \cdot e}{\phi_{max} \cdot K_c} \qquad (61)$$

where:

H = the total water column depth, ft

ϕ_{max} = the quantum yield, mg carbon fixed per mole of light quanta absorbed

K_e = the total extinction coefficient, computed from the sum of the non-algal light attenuation, K_e', and the self-shading attenuation due to ambient phytoplankton population, ft^{-1}

K_c = the extinction coefficient per unit of chlorophyll, m^2/mg chlorophyll-a

I_o = the incident light intensity at the surface, ly/day

θ = the ratio of carbon to chlorophyll in the phytoplankton, (mg carbon/mg chlorophyll-a)

e = the natural logarithm, 2.71828

As Smith (1980) points out, since the early experiments of Warburg and Negelein (1923), maximum photosynthetic quantum yield (ϕ_{max}) has been measured for a wide range of conditions (reviewed by Kok, 1960), and a nearly temperature-independent value of 0.08 to 0.1 mole O_2 per mole of photons absorbed is now widely accepted for photosynthesizing plants in general in the laboratory. Bannister (1974a) gives good arguments for adopting 0.06 mole carbon (0.07 mole O_2) per mole of photons as the maximum yield for plankton in nature. Reported values for K_c generally fall in the range 0.01 to 0.02 m^2mg^{-1}, and 0.016 m^2mg^{-1} has been suggested as the approximate average (Bannister, 1974b).

Equation 60 is an instantaneous rate and is numerically integrated over the day within the computer program to obtain daily growth, i.e.,

$$G(I) = \int_{o}^{1} \overline{G}_{1T}(t)dt \qquad 62$$

Equation 60 is quite similar to that formulated by Di Toro et al. (1971),

$$\overline{G}_{1T} = G_{1max}(T) \; . \; \frac{e \; . \; f}{K_e . H} \; . \; [\exp(\frac{-I_o}{I_s} e^{-K_e . H}) - \exp(\frac{-I_o}{I_s})] \qquad 63$$

except that the term I_s, the temperature-dependent light saturation parameter which is unknown and must be determined via the calibration-verification process, is replaced with a term involving the ratio of Φ_{max} and G_{1max}. The advantage of doing this is that both parameters, Φ_{max} and G_{1max}, are particularly well documented in the literature.

A second feature incorporated in the modeling framework derived from Smith's work is the calculation of a variable carbon to chlorophyll ratio based on the assumption that adaptive changes in carbon to chlorophyll occur so as to maximize the specific growth rate for ambient conditions of light and temperature. The expression used to calculate the carbon to chlorophyll ratio is presented in Equation 64:

$$\theta = \Phi_{max} \cdot K_c \cdot I_a / (G_{1max}(T) \cdot e) \qquad 64$$

where:

I_a = the average daily solar radiation, Ly/day.

A review of reported carbon/chlorophyll ratios in nature (Eppley and Sloane, 1966) suggests that physiological factors (in part the energy cost of synthesizing chlorophyll as compared with other cellular compounds) come into play to prevent θ from going much below 20, even in very low light. This lower limit of 20 has been included when determining a value for θ. Previously reported values of θ from algal composition studies conducted by EPA Region III's Central Regional Laboratory (CRL) are compared in Table 3 to calculated values of θ using Equation 64. There is general agreement between the measured and calculated values. Unfortunately, there are no winter algae composition studies available for comparison purposes.

TABLE 3. CARBON TO CHLOROPHYLL-A RATIO

Sampling Period	Carbon/Chlorophyll-a µg C/µg Chlor-a		
	Observed Mean	Observed Range	Predicted Range
July 20-Oct. 6, 1970[1]	45	25-68	24-28
August 1-29, 1977[2]	28	12-37	23-26
Sept. 7-28, 1978[2]	21	15-27	26-30
Sept. 7-28, 1978[3]		26-30	

1. Elemental analysis of blue-green algae
2. Laboratory elemental analysis of overall phytoplankton population
3. Estimates of cell composition based upon field data

The effects of various nutrient concentrations on the growth of phytoplankton have been investigated and the results are quite complex. As a first approximation to the effect of nutrient concentration on the growth rate, it is assumed that the phytoplankton population in question follows Monod growth kinetics with respect to the important nutrients. That is, at an adequate level of substrate concentration, the growth rate proceeds at the saturated rate for the ambient temperature and light conditions present. At low substrate concentration, however, the growth rate becomes linearly proportional to substrate concentration. Thus, for a nutrient with concentration N_j in the j^{th} segment, the factor by which the saturated growth rate is reduced in the j^{th} segment is: $N_j/(K_m + N_j)$. The constant, K_m (called the Michaelis or half-saturation constant) is the nutrient concentration at which the growth rate is half the saturated growth rate. Because there are two nutrients, nitrogen and phosphorus, considered in this framework, the Michaelis-Menton expression is evaluated for both nutrients and the minimum value is chosen to reduce the saturated growth rate,

$$G(N) = \text{Min}\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mp} + DIP}\right) \qquad 65$$

Figure 24 presents plots of G(N) versus DIN and DIP with $K_{mN} = 25$ µg-N/L and $K_{mP} = 1$ µg-P/L, respectively. The upper plot shows the standard Michaelis-Menton response curve to various concentrations of the inorganic nutrients. As can be seen, no significant reduction in growth rate is achieved until DIN is less than 200 µg/l (0.2 mg/l) or until DIP is less than 8 µg/l (0.008 mg/l).

The lower plot on Figure 24 uses an expanded nutrient scale and shows the Michaelis-Menton formulation in a slightly different format. Here the impact of the function may be evaluated quite readily. For example, a particular reach of the water body may have concentrations of DIN equal to 100 µg/l. This corresponds to a 20% reduction in the growth rate (G(N) = 0.8). In order for phosphorus to become the limiting nutrient in the same reach, dissolved inorganic phosphorus must reach a level of 4 µg/l or less. It should also be noted that if upstream nitrogen controls were instituted such that DIN was reduced to 60 µg/l for that same reach, then a further reduction in DIP to 2.5 µg/l would be required to keep phosphorus as the limiting nutrient. In other words, as water column concentrations of DIP begin to approach growth limiting levels due to continued reduction in point source phosphorus effluents, any nitrogen control strategies that might be instituted would require additional levels of phosphorus removal in order to keep phosphorus as the limiting nutrient.

Numerous mechanisms have been proposed that contribute to the death rate of phytoplankton: endogenous respiration, grazing by herbivorous zooplankton, sinking or settling from the water column and parasitization. The first three mechanisms have been included in previous models for phytoplankton dynamics, and they have been shown to be of general importance. If a large component of the algal biomass is comprised of blue-green algae that are not consumed upon by zooplankton, the zooplankton system may not need to be incorporated in the modeling framework.

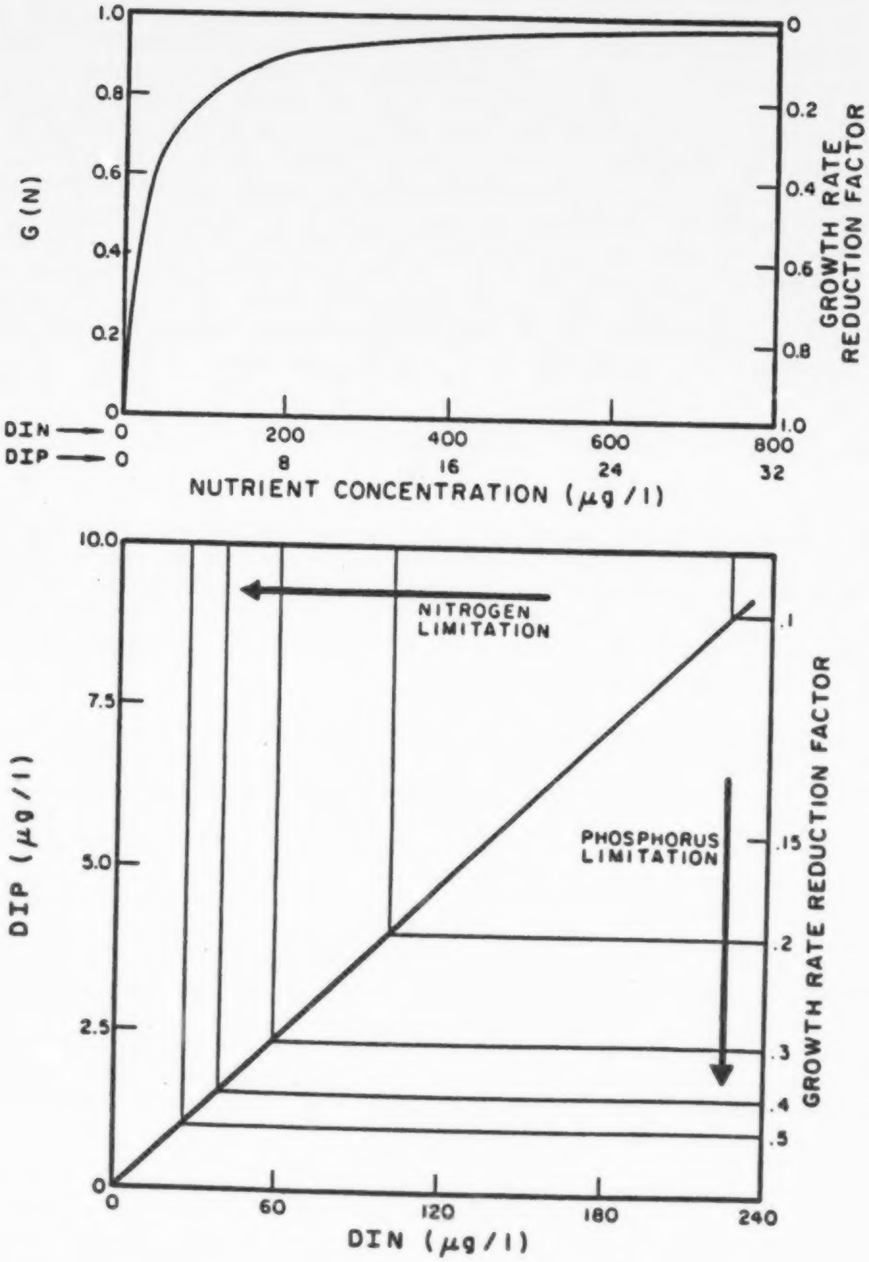


Figure 24. Effects of nutrient limitation on growth rate.

The endogenous respiration rate of phytoplankton is the rate at which the phytoplankton oxidize their organic carbon to carbon dioxide per unit weight of phytoplankton organic carbon. Respiration is the reverse of the photosynthesis process and, as such, contributes to the death rate of the phytoplankton population. If the respiration rate of the phytoplankton as a whole is greater than the growth rate, there is a net loss of phytoplankton carbon or biomass. The endogenous respiration rate is temperature dependent (Riley, 1949) and is determined via Equation 66:

$$k_{1R}(T) = k_{1R}(20°C) \cdot \Theta_{1R}^{T-20} \qquad 66$$

where:

$k_{1R}(20°C)$ = the endogenous respiration rate at 20°C, day^{-1}

$k_{1R}(T)$ = the temperature corrected rate, day^{-1}

Reported values of endogenous respiration at 20°C vary from 0.02 day^{-1} to 0.60 day^{-1}, with most values falling between 0.05 day^{-1} and 0.20 day^{-1} (Bowie et al., 1985). Di Toro and Matystik (1980) report a value of 1.045 for Θ_{1R}.

The settling of phytoplankton is an important contribution to the overall mortality of the phytoplankton population, particularly in lakes and coastal oceanic waters. Published values of the settling velocity of phytoplankton, mostly under quiescent laboratory conditions, range from 0.23-60 ft/day. In some instances, however, the settling velocity is zero or negative. Actual settling in natural waters is complex phenomenon, affected by vertical turbulence, density gradients, and the physiological state of the different species of phytoplankton. Although the effective settling rate of phytoplankton is greatly reduced in a relatively shallow well mixed river or estuary due to vertical turbulence, it still can contribute to the overall mortality of the algal population. In addition, the settling phytoplankton can be a significant source of nutrients to the sediments and can play an important role in the sediment oxygen demand. For these reasons, a term representing phytoplankton settling has been included in the algal mortality expression, and is determined by:

$$k_{s1j} = \frac{v_{s1}}{H_j} \qquad 67$$

where:

k_{s1j} = the effective algal settling or loss rate, day^{-1}

v_{s1} = the net settling velocity of phytoplankton from the water column to the sediment, ft/day

H_j = depth of the j th segment, ft

The total death rate for the phytoplankton in the j^{th} segment is expressed via Equation 68:

$$D_{1j} = k_{1R}(T) + k_{s1j} + k_{1D} \qquad 68$$

where:

D_{1j} = death rate, day^{-1}

k_{1D} = a non-predatory death rate, representing the effect of parasitization, i.e., the infection of algal cells by other microorganisms, and toxic materials, such as chlorine residual, day^{-1}

This completes the specification of the growth and death rates of the phytoplankton population in terms of the physical variables: light, temperature, and the nutrient concentrations present. (Table 4 summarizes these equations.) With these variables known as a function of time, it is possible to calculate the phytoplankton chlorophyll throughout the year. The nutrients are not known a priori, however, because they depend upon the phytoplankton population that develops. That is, these systems are interdependent and cannot be analyzed separately. It is necessary to formulate a mass balance for the nutrients as well as the phytoplankton in order to calculate the chlorophyll that would develop for a given set of environmental conditions.

1.4.3 Stoichiometry and Uptake Kinetics

A principal component in the mass-balance equations written for the nutrient systems included in the eutrophication framework is the nutrient uptake kinetics associated with algal growth. To specify the nutrient uptake kinetics associated with this growth, however, it is necessary to specify the population stoichiometry in units of nutrient uptake/mass of population synthesized. For carbon as the unit of population biomass, the relevant ratios are the mass of nitrogen and phosphorus per unit mass of carbon. A selection of these ratios presented (Di Toro et al., 1971) indicates that their variability is quite large. The use of constant ratios in the analysis, then, is questionable.

Upon further investigation, however, it is clear that the reason these ratios vary is the varying cellular content of nutrients, which is, in turn, a function of the external nutrient concentrations and the past history of the algal population. Large ratios of carbon to nitrogen or phosphorus correspond to that nutrient limiting growth; small ratios reflect excess nutrients. Thus, the choice of the relevant ratios can be made with the specific situation in mind.

The operational consequence of this choice is that the population stoichiometry under non-limiting conditions may be underestimated, but under limiting conditions should be estimated correctly. Hence the tradeoff is a probable lack of realism during a portion of the year versus a correct estimate of algal biomass during periods of possible nutrient limitations. Because this is usually the critical period and because

TABLE 4. PHYTOPLANKTON NET GROWTH EQUATION

$$S_{1_j} = G_{1max}(T) \cdot G(I) \cdot G(N) - k_{1R}\theta_{1R}^{T-20} - \frac{V_{s1}}{H} - k_{1D}$$

Temperature Correction

$$G_{1max}(T) = G_{1max}\theta_1^{T-20}$$

Light Reduction

$$G(I) = \frac{e}{K_e \cdot H} \int_o^1 (e^{-\alpha_1} - e^{-\alpha_0})dt$$

$$\alpha_1 = \frac{\Phi_{max}\ K_C\ I_o(t)}{G_{1max}(T)\theta \exp(1+K_e.H)} \qquad \alpha_o = \frac{\Phi_{max} \cdot K_C \cdot I_o(t)}{G_{1max}(T)\theta \cdot e}$$

$$\theta = \text{Carbon/Chlorophyll Ratio} = \frac{\Phi_{max} \cdot K_C \cdot I_o(t)}{G_{1max}(T) \cdot e}$$

Nutrient Uptake

$$G(N) = \text{Min}\left(\frac{[DIN]}{K_{mN} + [DIN]}, \frac{[DIP]}{K_{mP} + [DIP]}\right)$$

[DIN] = dissolved inorganic nitrogen = $[NH_3\text{-}N] + [NO_3\text{-}N]$

[DIP] = disolved inorganic phosphorus

TABLE 4. PHYTOPLANKTON NET GROWTH EQUATION (Continued)

Exogenous Variables

Description	Notation
Extinction Coefficient	K_e
Segment Depth	H or d (in Figures)
Instantaneous Surface Solar Radiation	$I_o(t)$
Average Daily Surface Solar Radiation	I_a
Temperature	T
Time	t

Rate Constants

Description	Notation	Value Used in the Potomac River Study	Units
Maximum Specific Growth Rate @ 20°C	G_{1max}	2.0	day^{-1}
Temperature Coefficient	θ_1	1.068	none
Maximum Photosynthetic Quantum Yield	Φ_{max}	720.0	$\frac{mg\ C}{mole\ photon}$
Phytoplankton Self-Light Attenuation	K_c	0.017	m^2/mg Chl 'a'
Half-Saturation Constant for Nitrogen	K_{mN}	25.0	µg N/1
Half-Saturation Constant for Phosphorus	K_{mP}	1.0	µg P/1
Algal Endogenous Respiration	k_{1R}	0.125	day^{-1}
Temperature Coefficient	θ_{1R}	1.045	none
Algal Settling Rate	v_{s1}	0.3	ft/day
Non-Predatory Death	k_{1D}	0.02	day^{-1}

most questions to be answered are usually sensitive to maximum summer populations, this choice is a practical expedient. A comparison of carbon-to-nitrogen and carbon-to-phosphorus ratios measured in the Potomac Estuary is provided in Table 5.

TABLE 5. PHOSPHORUS-TO-CARBON AND NITROGEN-TO-CARBON RATIOS

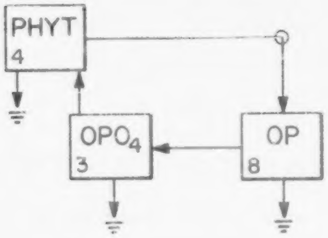
	Phosphorus/Carbon mg P/mg C		Nitrogen/Carbon mg N/mg C	
Sampling Period	Observed Mean	Observed Range	Observed Mean	Observed Range
July 20-Oct. 6, 1970[1]	0.023	0.010-0.046	0.26	0.10-0.48
August 1-29, 1977[2]	0.024	0.012-0.028	0.24	0.15-0.36
Sept. 7-28, 1978[2]	0.030	0.017-0.047	0.26	0.18-0.35
Sept. 7-28, 1978[3]	0.031		0.26	
Model	0.025		0.25	

1. Elemental analysis of blue-green algae
2. Laboratory elemental analysis of overall phytoplankton population
3. Estimates of cell composition based upon field data

Once the stoichiometric ratios have been determined, the mass balance equations may be written for the nutrients in much the same way as is done for the phytoplankton biomass. The primary interaction between the nutrient systems and the phytoplankton system is the reduction or sink of nutrients associated with phytoplankton growth. A secondary interaction occurs wherein the phytoplankton system acts as a source of nutrients due to release of stored cellular nitrogen and phosphorus during algal respiration and death.

1.4.4 The Phosphorus Cycle

Three phosphorus state variables are modeled: phytoplankton phosphorus, organic phosphorus, and inorganic (orthophosphate) phosphorus. A summary is illustrated in Figure 25. Organic phosphorus is divided into particulate and dissolved concentrations by a user-specified fraction. Inorganic phosphorus also is divided into particulate and dissolved concentrations by spatially variable fractions, reflecting sorption. Table 6 presents the reaction rate terms used in the Potomac study. A fraction of the phosphorus



4. PHYTOPLANKTON PHOSPHORUS

$$\frac{\partial(C_4\cdot a_{PC})}{\partial t} = \Big(\underbrace{GPI}_{\text{growth}} - \underbrace{DPI}_{\text{death}} - \underbrace{\frac{SVPI}{d}}_{\text{settling}}\Big)\cdot C_4\cdot a_{PC}$$

8. ORGANIC PHOSPHORUS

$$\frac{\partial C_8}{\partial t} = \underbrace{+DPI\cdot C_4\cdot a_{PC}}_{\text{death}} - \underbrace{K_{83}\theta_{83}^{T-20}\cdot X_{PRC}\cdot C_8}_{\text{mineralization}} - \underbrace{\frac{SVPP\cdot f_{SOP}}{d}\cdot C_8}_{\text{settling}}$$

3. ORTHOPHOSPHATE PHOSPHORUS

$$\frac{\partial C_3}{\partial t} = \underbrace{+K_{83}\theta_{83}^{T-20}\cdot X_{PRC}\cdot C_8}_{\text{mineralization}} - \underbrace{GPI\cdot C_4\cdot a_{PC}}_{\text{growth}} - \underbrace{\frac{SVPP\cdot f_{PIP}^{(x)}}{d}\cdot C_3}_{\text{settling}}$$

$$X_{PRC} = \frac{C_4}{K_{mPC} + C_4} \quad \text{Phytoplankton affects mineralization}$$

Figure 25. Phosphorus cycle

released during phytoplankton respiration and death is in the inorganic form and readily available for uptake by other viable algal cells. In work on the Great Lakes this fraction was assigned at 50% (Di Toro and Matystik, 1980).

The remaining fraction released is in the organic form and must undergo a mineralization or bacterial decomposition into inorganic phosphorus before utilization by phytoplankton. In their work on Lake Huron and Saginaw Bay, Di Toro and Matystik (1980) proposed a nutrient recycle formulation that was a function of the localized phytoplankton population. Drawing from an analysis of available field data and citing the work of others (Hendry, 1977;

TABLE 6. PHOSPHORUS REACTION TERMS

Description	Notation	Value	Units
Phytoplankton biomass	P_C	-	mg C/1
Specific phytoplankton growth rate	G_{1j}	*	day^{-1}
Phosphorus to carbon ratio	a_{PC}	0.025	mg P/mg C
Dissolved organic phosphorus mineralization at 20°C	k_{58}	0.22	day^{-1}
Temperature coefficient	θ_{58}	1.08	none
Particulate organic phosphorus mineralization rate at 20°C	k_{68}	0.22	day^{-1}
Temperature coefficient	θ_{68}	1.08	none
Fraction of dead and respired phytoplankton recycled ...			
to the dissolved organic phosphorus pool	f_{DOP}	0.10	none
to the particulate organic phosphorus pool	f_{POP}	0.4	none
to the dissolved inorganic phosphorus pool	f_{DIP}	0.5	none
Half saturation constant for phytoplankton limitation	K_{mPc}	1.0	mg C/1
Fraction particulate inorganic phosphorus in the water column	f_{pwc}	0.15 0.30	none

* $G_{1j} = G_{1max}(T) \cdot G(I) \cdot G(N)$

(Hendry, 1977; Lowe, 1976; Henrici, 1938; Menon, 1972; and Rao, 1976) that indicated bacterial biomass increased as phytoplankton biomass increased. The mechanism chosen, saturating recycle, was a compromise between the conventional first-order, temperature-corrected mechanism, and a second order recycle mechanism wherein the recycle rate is directly proportional to the phytoplankton biomass present, as had been indicated in pure culture, bacteria seeded, laboratory studies (Jewell and McCarty, 1971). The various relationships may be written:

First order recycle: $k(T) = k'(20°C)\theta^{T-20}$ 69

Second order recycle: $k(T) = k'(20°C)\theta^{T-20} \cdot P_c$ 70

Saturating recycle: $k(T) = k'(20°C)\theta^{T-20} \cdot \frac{P_c}{K_{mPc} + P_c}$ 71

Saturating recycle permits second order dependency at low phytoplankton concentrations, when $P_c << K_{mPc}$, where K_{mPc} is the half-saturation constant for recycle, and permits first order recycle when the phytoplankton greatly exceed the half-saturation constant. Basically this mechanism slows the recycle rate if the algal population is small but does not permit the rate to increase continuously as phytoplankton increase. The assumption is that at higher population levels other factors are rate limiting the recycle kinetics so that it proceeds at its maximum first order rate.

There is an adsorption-desorption interaction between dissolved inorganic phosphorus, and suspended particulate matter in the water column. The subsequent settling of the suspended solids together with the sorbed inorganic phosphorus can act as a significant loss mechanism in the water column and is a source of phosphorus to the sediment. Because sufficient suspended solids data were not available to provide for a calibration and verification analysis of suspended solids as a state variable, an alternate formulation to the adsorption-desorption kinetics was required. This alternate formulation takes advantage of the fact that the rates of reaction for adsorption-desorption are in the order of minutes versus reaction rates in the order of days for the algal and biological kinetics, and so permits an "instantaneous equilibrium" assumption to be made. Instantaneous equilibrium implies that the dissolved and particulate phosphorus phases "instantaneously" react to any discharge sources of phosphorus or runoff or shoreline erosion of solids so as to redistribute the phosphorus to its "equilibrium" dissolved and solids phase concentrations.

Consider C_{DIP} to be the concentration of dissolved inorganic phosphorus in the water column. It interacts with the particulate concentration, C_{PIP}. The interaction may be an adsorption-desorption process with the solids or an assimilation-depuration process with the phytoplankton. If the total suspended solids (inorganic solids plus phytoplankton solids) is considered, the particulate concentration can be defined as:

$C_{PIP} = C'_{PIP} \cdot S$ 72

where:

C'_{PIP} = concentration of phosphorus sorbed to suspended solids, mgP/Kg SS

S = concentration of suspended solids, Kg/L

The total inorganic phosphorus is then the sum of dissolved inorganic and the particulate inorganic phosphorus

$$C_{TIP} = C_{DIP} + C_{PIP} \qquad 73$$

The underlying assumption that is made, as mentioned previously, is "instantaneous equilibrium" between the adsorption-desorption process. The equilibrium between the dissolved inorganic phosphorus in the water column and the mass concentration of inorganic phosphorus of the solids is usually expressed in terms of a partition coefficient:

$$K_{PIP} = \frac{C'_{PIP}}{C_{DIP}} \qquad 74$$

where:

K_{PIP} = partition coefficient for particulate phosphorus, mgP/Kg S per (mg P/L) or (L/Kg S)

$$C_{PIP} = K_{PIP} \cdot S \cdot C_{DIP} \qquad 75$$

Equation 75 is the linear portion of the Langmuir isotherm. Although not always representative of actual conditions, it is a reasonable approximation when (mgP_{sorbed}/KgS) per ($mgP_{dissolved}$/L) or (L/KgS) is much less than the ultimate adsorbing capacity of the solids. Combining Equations 73 and 75, the total concentration may be expressed as

$$C_{TIP} = C_{DIP} + K_{PIP} \cdot S \cdot C_{DIP} \qquad 76$$

The dissolved and particulate fractions may be expressed, respectively, as

$$f_{DIP} = \frac{C_{DIP}}{C_{TIP}} = \frac{1}{1 + K_{PIP} \cdot S} \qquad 77$$

$$f_{PIP} = \frac{C_{PIP}}{C_{TIP}} = \frac{K_{PIP} \cdot S}{1 + K_{PIP} \cdot S} \qquad 78$$

A wide range of partition coefficients is found in the literature. Thomann and Fitzpatrick (1982) report values between 100 and 1600. Using a range in partition coefficients from 1,000 - 16,000 and a range of inorganic solids of from 10 to 30 mg/l in the water column leads to a range in the fraction particulate inorganic phosphorus of from 0.01 to 0.33.

The mechanism incorporated in the model framework for computing dissolved and sorbed phosphorus sacrifices some degree of realism for computational simplicity. Essentially the dissolved and particulate phosphorus phases are assigned as fixed fractions of the total inorganic phosphorus. Internally the computation is performed as follows: at the beginning of each computational step in the integration procedure for each segment in the model, the total inorganic phosphorus is computed as the sum of the dissolved and sorbed inorganic phosphorus in that segment, and then redistributed to the dissolved phase, for algal uptake, and the particulate phase, for settling, using an assigned fraction for each phase. The computational steps may be written:

$$TIP = DIP_{t-1} + PIP_{t-1} \qquad 79$$

$$PIP = f_p \cdot TIP \qquad 80$$

$$DIP = (1 - f_p) \cdot TIP \qquad 81$$

where:

TIP = the total inorganic phosphorus, mg/L

DIP_{t-1} = the dissolved inorganic phosphorus resulting from the previous integration step, mg/L

PIP_{t-1} = the sorbed inorganic phosphorus resulting from the previous integration step, mg/L

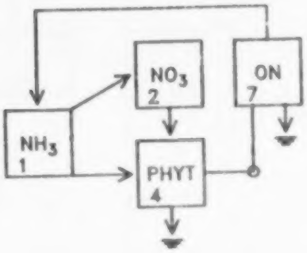
f_p = the fraction of the total inorganic phosphorus assigned to the sorbed or particulate phase, unitless

DIP = the new "equilibrium" dissolved inorganic phosphorus, available for algal uptake is the new "equilibrium" sorbed inorganic phosphorus, which may then settle to the sediment layer from the water column, mg/L.

1.4.5 The Nitrogen Cycle

Four nitrogen state variables are modeled: phytoplankton nitrogen, organic nitrogen, ammonia, and nitrate. A summary is illustrated in Figures 26 and 27. The kinetic structure for nitrogen is similar to that for the phosphorus system. Table 7 summarizes the terms used in the nitrogen system kinetics. During algal respiration and death, a fraction of the cellular nitrogen is returned to the inorganic pool in the form of ammonia nitrogen. The fraction recycled to the inorganic pool for Great Lakes models has been assigned at 50% (DiToro and Matystik, 1980). The remaining fraction is recycled to the organic nitrogen pool. Organic nitrogen undergoes a bacterial decomposition whose end-product is ammonia nitrogen. Ammonia nitrogen, in the presence of nitrifying bacteria and oxygen, is converted to nitrate nitrogen (nitrification). Both ammonia and nitrate are available for uptake and use in cell growth by phytoplankton; however, for physiological reasons, the preferred form is ammonia nitrogen. The ammonia preference term takes the following form.

$$\alpha_{NH_3} = NH_3 \cdot \frac{NO_3}{(K_{mN}+NH_3)(K_{mN}+NO_3)} + NH_3 \cdot \frac{K_{mN}}{(NH_3+NO_3)(K_{mN}+NO_3)} \qquad (82)$$



1. AMMONIA NITROGEN

$$\frac{dC_1}{dt} = \underset{\text{mineralization}}{+K_{71}\theta_{71}^{T-20}\, X_{PRC} \cdot C_7} - \underset{\text{growth}}{GPI \cdot P_{NH_3} \cdot C_4 \cdot a_{NC}}$$

$$\underset{\text{nitrification}}{-K_{12}\theta_{12}^{T-20} \cdot \left(\frac{C_6}{K_{NIT} + C_6}\right) \cdot C_1}$$

2. NITRATE NITROGEN

$$\frac{dC_2}{dt} = \underset{\text{nitrification}}{+K_{12}\theta_{12}^{T-20} \cdot \left(\frac{C_6}{K_{NIT} + C_6}\right) \cdot C_1} - \underset{\text{growth}}{GPI \cdot (1 - P_{NH_3}) \cdot C_4 \cdot a_{NC}}$$

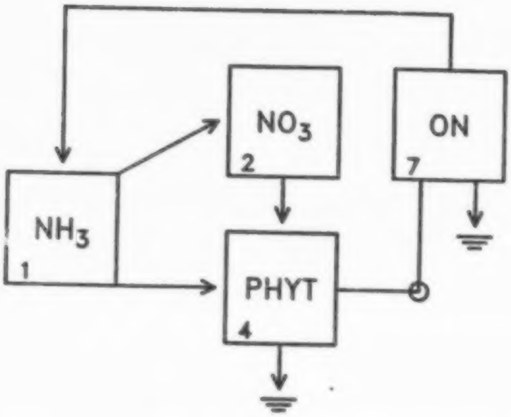
$$\underset{\text{denitrification}}{-K_{2D}\theta_{2D}^{T-20} \cdot \left(\frac{K_{NO_3}}{K_{NO_3} + C_6}\right) \cdot C_2}$$

$$\underset{\text{ammonia preference factor}}{P_{NH_3} = C_1 \cdot \frac{C_2}{(K_{mN} + C_1)\,(K_{mN} + C_2)} + C_1 \cdot \frac{K_{mN}}{(C_1 + C_2)\,(K_{mN} + C_2)}}$$

Figure 26. Nitrogen cycle.

The behavior of this equation, for a Michaelis value, K_{mN}, of 25 μg N/1, is shown in Figure 28. The behavior of Equation 82 is most sensitive at low values of ammonia or nitrate. For a given concentration of ammonia, as the available nitrate increases above approximately the Michaelis limitation, the preference for ammonia reaches an asymptote. Also as the concentration of available ammonia increases, the plateau levels off at values closer to unity, i.e., total preference for ammonia.

The process of nitrification in natural waters is carried out by aerobic autotrophs; Nitrosomonas and Nitrobacter predominate in fresh waters. It is a two-step process with Nitrosomonas bacteria responsible for the conversion of ammonia to nitrite and Nitrobacter responsible for the conversion of nitrite



4. PHYTOPLANKTON NITROGEN

$$\frac{d(C_4 \cdot a_{NC})}{dt} = \left(GPI - DPI - \frac{SVPI}{d}\right) \cdot C_4 \cdot a_{NC}$$

growth death settling

7. ORGANIC NITROGEN

$$\frac{dC_7}{dt} = +DPI \cdot C_4 \cdot a_{N}C - K_{71}\theta_{71}^{T-20} \cdot X_{PRC} \cdot C_7 - \frac{SVPN \cdot f_{SON}}{d} \cdot C_7$$

death mineralization settling

Figure 27. Nitrogen cycle.

to nitrate. Essential to this reaction process are aerobic conditions. Also this process appears to be affected by high or low values of pH that inhibit Nitrosomonas growth, particularly for pH below 7 and greater than 9. Anthonsien et al. (1976) postulates that the existence of free ammonia and nitrous acid inhibits nitrifying organisms by causing differences between intercellular and extracellular pH.

As with phytoplankton, the nitrifying bacterial populations are sensitive to flow. During periods of high flow or storm runoff, upstream bacteria may be advected downstream, with some lag time after a flow transient before they can build up to significant levels again.

Therefore, the process of nitrification in natural waters is a complex phenomenon depending on dissolved oxygen, pH, and flow conditions, which in turn leads to spatially and temporally varying rates of nitrification. To properly account for this complex phenomenon in the modeling framework would require an additional five state variables: nitrite, Nitrosomonas

TABLE 7. NITROGEN REACTION TERMS

Description	Notation	Value from Potomac Estuary Model	Units
Nitrogen to carbon ratio	a_{NC}	0.25	mg N/mg C
Organic nitrogen mineralization rate @ 20°C	k_{1013}	0.075	day^{-1}
Temperature coefficient	θ_{1013}	1.08	none
Nitrification rate @ 20°C	k_{1314}	0.09	day^{-1}
		0.13	
Temperature coefficient	θ_{1314}	1.08	none
Half saturation constant for oxygen limitation	K_{nit}	2.0	mg O_2/ℓ
Denitrification rate @ 20°C	k_{140}	0.09	day^{-1}
Temperature coefficient	θ_{140}	1.045	none
Michaelis constant for denitrification	K_{NO_3}	0.1	mg O_2/ℓ
Fraction of dead and respired phytoplankton recycled...			
to the organic nitrogen pool	f_{ON}	0.5	none
to the ammonia nitrogen pool	f_{NH_3}	0.5	none
Preference for ammonia uptake term	α_{NH_3}	cf. Eq. 82	none

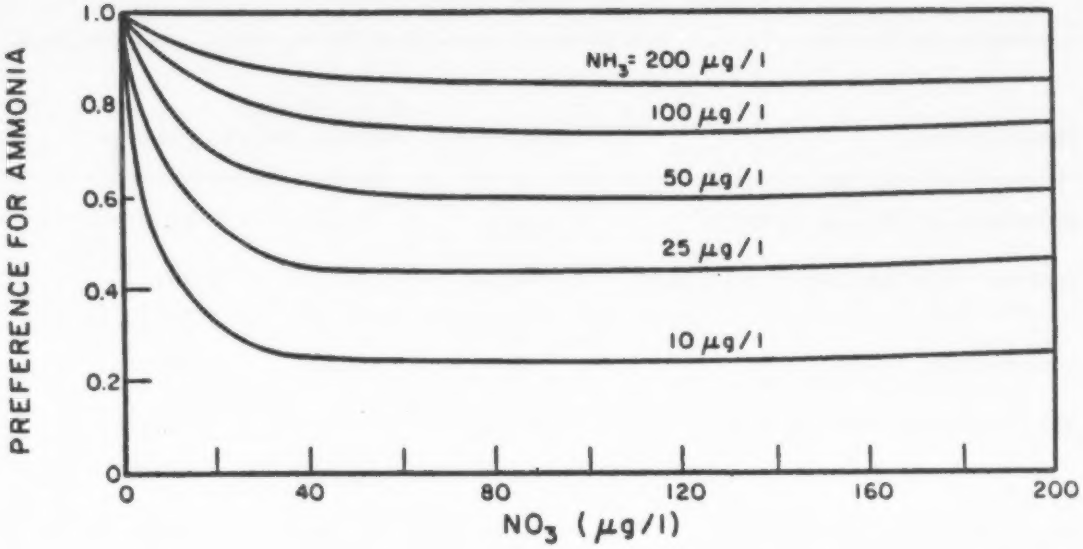


Figure 28. Ammonia preference structure (Thomann and Fitzpatrick 1982).

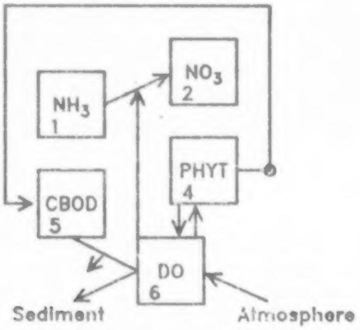
and Nitrobacter bacteria, and total inorganic carbon and alkalinity from which to calculate pH. Unfortunately, the data base to support the calibration/verification of these additional state variables is usually unavailable. Therefore, the process of nitrification is of necessity reduced to a simple spatially invariant, but temperature-corrected, first-order reaction rate.

Denitrification refers to the reduction of NO_3 (or NO_2) to N_2 and other gaseous products such as N_2O and NO. This process is carried out by a large number of heterotrophic, facultative anaerobes. Under normal aerobic conditions found in the water column, these organisms use oxygen to oxidize organic material. Under the anaerobic conditions found in the sediment bed or during extremely low oxygen conditions in the water column, however, these organisms are able to use NO_3 as the electron acceptor.

The process of denitrification is included in the modeling framework simply as a sink of nitrate. This process is assumed to always occur in the sediment layer where anaerobic conditions always exist. In the water column, however, denitrification should occur only under extremely low dissolved oxygen conditions. This is accomplished computationally by modifying the linear first-order denitrification rate by the expression $K_{NO3}/(K_{NO3} + DO)$. This expression is similar to the Michaelis - Menton expression, and for concentrations of DO greater than 1 mg/l, this expression reduces denitrification to near zero, whereas for DO levels less than 0.1 mg/l this expression permits denitrification to occur.

1.4.6 The Dissolved Oxygen Balance

Five state variables participate in the DO balance: phytoplankton carbon, ammonia, nitrate, carbonaceous biochemical oxygen demand, and dissolved oxygen. A summary is illustrated in Figure 29. The reduction of dissolved oxygen is a consequence of the aerobic respiratory processes in the water column and the anaerobic processes in the underlying sediments. Both these processes contribute significantly and, therefore, it is necessary to formulate their kinetics explicitly.



5. CARBONACEOUS BOD

$$\frac{dC_5}{dt} = \underbrace{KID \cdot C_4 \cdot a_{OC}}_{\text{death}} \underbrace{- K_D \theta_D^{T-20} \cdot C_5 \cdot \frac{C_6}{K_{BOD} + C_6}}_{\text{oxidation}} - \underbrace{\frac{SVBOD}{d}}_{\text{settling}} \cdot C_5$$

$$\underbrace{- \frac{5}{4} \cdot \frac{32}{14} \cdot K_{2D} \cdot \theta_{2D}^{T-20} \cdot \left(\frac{K_{NO_3}}{K_{NO_3} + C_6} \right) \cdot C_2}_{\text{denitrification}}$$

6. DISSOLVED OXYGEN

$$\frac{dC_6}{dt} = \underbrace{K_A \theta_A^{T-20} (C_S - C_6)}_{\text{reaeration}} - \underbrace{K_D \theta_D^{T-20} \cdot C_5 \cdot \left(\frac{C_6}{K_{BOD} + C_6} \right)}_{\text{oxidation}}$$

$$\underbrace{- \frac{64}{14} \cdot K_{12} \theta_{12}^{T-20} \cdot \left(\frac{C_6}{K_{NIT} + C_6} \right) \cdot C_1}_{\text{nitrification}} - \underbrace{RESP \cdot a_{OC}}_{\text{respiration}} - \underbrace{\frac{SOD}{d}}_{\text{sediment}}$$

$$\underbrace{+ GPI \cdot C_4 \cdot \left(\frac{32 \cdot P_{NH_3}}{12} + \frac{1.5 \cdot a_{NC}}{14} (1 - P_{NH_3}) \right)}_{\text{growth using } CO_2,\ NH_3,\ NO_3 \text{ (photosynthesis)}}$$

Figure 29. Oxygen balance.

The methodology for the analysis of dissolved oxygen dynamics in natural waters, particularly in streams, rivers, and estuaries is reasonably well-developed (O'Connor and Thomann, 1972). The long history of applications have focused primarily on the use of biochemical oyxgen demand (BOD) as the measure of the quantity of oxygen-demanding material and its rate of oxidation as the controlling kinetic reaction. This has proven to be appropriate for waters receiving a heterogeneous combination of organic wastes of municipal and industrial origin since an aggregate measure of their potential effect is a great simplification that reduces a complex problem to one of tractable dimensions.

A byproduct of photosynthetic carbon fixation is the production of dissolved oxygen. The rate of oxygen production (and nutrient uptake) is proportional to the growth rate of the phytoplankton since its stoichiometry is fixed. An additional source of oxygen from algal growth occurs when the available ammonia nutrient source is exhausted and the phytoplankton begin to utilize the available nitrate. For nitrate uptake the initial step is a reduction to ammonia which produces oxygen as shown in equation 83:

$$2NO_3 \rightarrow 2NH_3 + 3O_2 \qquad 83$$

Oxygen deficient, i.e., below saturation, waters are replenished via atmospheric reaeration. The reaeration coefficient is a function of the average water velocity, depth, wind, and temperature. EUTRWASP calculates flow-induced reaeration based on the Covar method (Covar, 1976). This method calculates reaeration as a function of velocity and depth by one of three formulas, Owens, Churchill, or O'Connor-Dobbins, respectively:

$$k_{aj}(20°C) = 21.7 \cdot V_{tj}^{0.67} \cdot H_j^{-1.85} \qquad 84$$

$$k_{aj}(20°C) = 11.7 \cdot V_{tj}^{0.97} \cdot H_j^{-1.67} \qquad 85$$

or $$k_{aj}(20°C) = 12.9 \cdot V_{tj}^{0.50} \cdot H_j^{-1.50} \qquad 86$$

where:

K_{aj} = reaeration rate coefficient at 20°C, day^{-1}

V_{tj} = average water velocity in segment j, ft/sec

H_j = average segment depth, ft

The Owens formula is automatically selected for segments with depth less than 2 feet. For segments deeper than 2 feet, the O'Connor-Dobbins or Churchill formula is selected based on a consideration of depth and velocity. Deeper, slowly moving rivers require O'Connor-Dobbins; moderately shallow, faster moving streams require Churchill.

Wind-induced reaeration is determined by

$$k_{aj}(20°C) = 0.46 \cdot W + 0.136 \cdot W^2 \qquad 87$$

where:

W = time-varying windspeed at 10 cm above surface, m/sec

A minimum value of $1.6/H_j$ day^{-1} is imposed on $k_{aj}(20°C)$. Windspeed affects reaeration, then, above 6 meters/sec. The reaeration velocity used to compute volatilization is either the flow-induced reaeration or the wind-induced reaeration, whichever is larger. Segment temperatures are used to adjust $k_{aj}(20°C)$ by the standard formula:

$$k_{aj}(T) = k_{aj}(20°C)\ \theta_a^{T-20} \qquad 88$$

where:

T = temperature, °C

$k_{aj}(T)$ = reaeration rate coefficient at ambient segment temperature, day^{-1}

θ_a = temperature coefficient, unitless

Dissolved oxygen saturation is determined as a function of temperature:

$$DO_{sat} = 14.652 - 0.41022.T + 0.007991.T^2 - 0.00007777.T^3 \qquad 89$$

Oxygen is diminished in the water column as a result of algal respiration, which is basically the reverse process of photosynthesis:

$$C_4 + (\frac{12}{32} \cdot a_{oc})\ O_2 \longrightarrow CO_2 \qquad 90$$

where:

C_4 = phytoplankton carbon, mg/L

a_{oc} = oxygen to carbon ratio for phytoplankton espiration, gO_2/gC_4

Additional losses of oxygen occur as a result of nitrification:

$$NH_3^+ + 2O_2 \rightarrow NO_3 + H_2O + H^+ \qquad 91$$

and of oxidation of carbonaceous material (including detrital phytoplankton). These three reactions together with sediment oxygen demand (to be detailed below) account for the loss of oxygen in the water column.

The oxidation of carbonaceous material is the classical BOD reaction. Internally the model uses ultimate carbonaceous biochemical oxygen demand CBOD as the indicator of equivalent oxygen demand for the carbonaceous material. The principal source of CBOD, other than man-made sources and natural runoff, is detrital phytoplankton carbon, produced as a result of algal death. The loss mechanisms associated with CBOD are oxidation

$$C_xH_yO_z \rightarrow CO_2 + H_2O \tag{92}$$

and denitrification

$$5CH_2O + 5H_2O + 4NO_3 + 4H^+ \rightarrow 5CO_2 + 2N_2 + 12H_2O \tag{93}$$

although the latter is not a significant loss in the water column.

Direct comparisons between observed BOD_5 data and model output cannot be made using the internal $CBOD_5$ computed by EUTRWASP, since field measurements may be tainted by algal respiration and the decay of algal carbon. Therefore a correction must be made to the internally computed model $CBOD_5$ so that a valid comparison to the field measurement may be made. This results in a new variable, known as the bottle BOD_5, which is computed via equation 94.

$$\text{Bottle } BOD_5 = CBOD_5 + a_{oc}P_c(1-e^{5 \cdot k_{1R}(T)}) \tag{94}$$

where:

$CBOD_5$ = the internally computed 5-day CBOD, mg/L

a_{oc} = the oxygen to carbon ratio, mg O_2/mg C

P_c = the phytoplankton biomass in carbon units, mg/L

$k_{1R}^{(T)}$ = the algal respiration rate at 20°C, the temperature at which the field samples were incubated, day^{-1}

Note that Equation 94 is a conservative estimate of the observed bottle BOD because it does not include a correction for the decay of detrital algal carbon, which in turn depends upon the number of non-viable phytoplankton. Also, Equation 94 may tend to underestimate observed bottle BODs if a nitrifying inhibitor is not used before setting the BODs. Therefore, depending upon environmental conditions in the water body from which the samples were taken, some oxygen utilization may be occurring in the bottle due to nitrification, which is not included in the internal computation of bottle BOD by EUTRWASP. Therefore, it is reasonable to expect that the model will underestimate bottle BOD.

Table 8 summarizes the water column CBOD and DO reaction rates. The formulation for the sediment reactions require a more detailed explanation of the sediment mass transport and kinetics and these are presented subsequently.

1.4.7 Sediment - Water Interactions

The decomposition of organic material in benthic sediment can have profound effects on the concentrations of oxygen and nutrients in the overlying waters. The decomposition of organic material releases nutrients to the sediment interstitial waters and also results in the exertion of an oxygen demand at the sediment-water interface. As a result, the areal fluxes

TABLE 8. CBOD AND DO REACTION RATES

Carbonaceous Biochemical Oxygen Demand

$$S_{18j} = a_{OC}k_{1D}[P_c] - k_d\theta_d^{T-20}[CBOD]\ \frac{[DO]}{K_{BOD} + [DO]}$$

$$- 5/4\ a_{ON}\ k_{140}\theta_{140}^{T-20}[NO_3]\ \left(\frac{K_{NO_3}}{K_{NO_3} + [DO]}\right)$$

Dissolved Oxygen

$$S_{19j} = a_{OC}G_{1j}[P_c] + (a_{NO_3C})(1 - \alpha_{NH_3})G_{1j}[P_c] + k_a\theta_a^{T-20}(DO_{sat} - [DO])$$

$$- a_{OC}\ k_{1R}\theta_{1R}^{T-20}[P_c] - 2\ a_{ON}\ k_{1314}\theta_{1314}^{T-20}[NH_3]\ \frac{[DO]}{K_{nit} + [DO]}$$

$$- k_d\theta^{T-20}[CBOD]\ \frac{[DO]}{K_{BOD} + [DO]}$$

TABLE 8. CBOD AND DO REACTION RATES (Continued)

Rate Constants

Description	Notation	Value from Potomac Estuary Model	Units
Oxygen to carbon ratio	a_{OC}	32/12	mg O_2/mg C
Ratio of the ultimate to 5-day carbonaceous biochemical oxygen demand	BOD_{U5}	1.85	none
Deoxygenation rate @ 20°C	k_d	0.21	day^{-1}
		0.16	
Temperature coefficient	θ_d	1.047	none
Half saturation constant for oxygen limitation	K_{BOD}	0.5	mg O_2/l
Oxygen to nitrogen ratio	a_{ON}	32/14	mg O_2/mg N
Oxygen to carbon ratio for nitrate uptake	a_{NO_3C}	$(\frac{48}{14})a_{NC}$	mg O_2/mg C
Reaeration rate @ 20°C	k_a	cf Eq. 84-87	day^{-1}
Temperature coefficient	θ_a	1.028	none
Dissolved oxygen saturation	DO_{sat}	cf Eq. 40	mg O_2/l

from the sediment can be substantial nutrient sources or oxygen sinks, on a volumetric basis, to the overlying water column. Additionally, the occurrence of anoxia, due in part to the sediment oxygen demand, may dramatically increase certain nutrient fluxes. The details of the mechanisms responsible for this increase are as yet unclear but they are related to a set of complex redox reactions that change the state and concentrations of various nutrients and metals thereby releasing bound nutrients. The relative importance of the sediment oxygen demand and nutrient fluxes vis-a-vis future nutrient control strategies requires the incorporation of a dynamic sediment layer and its associated interactions with the overlying water column in a framework that is consistent with that discussed in the previous sections.

This model provides two options for nutrient and oxygen fluxes: descriptive input and predictive calculations (Fig. 30). The first option is used for networks composed of water column segments only. Observed fluxes and surface areas must be specified for ammonia, phosphate, and dissolved oxygen (i.e., sediment oxygen demand). Time functions may be specified for ammonia and phosphate, reflecting seasonal changes.

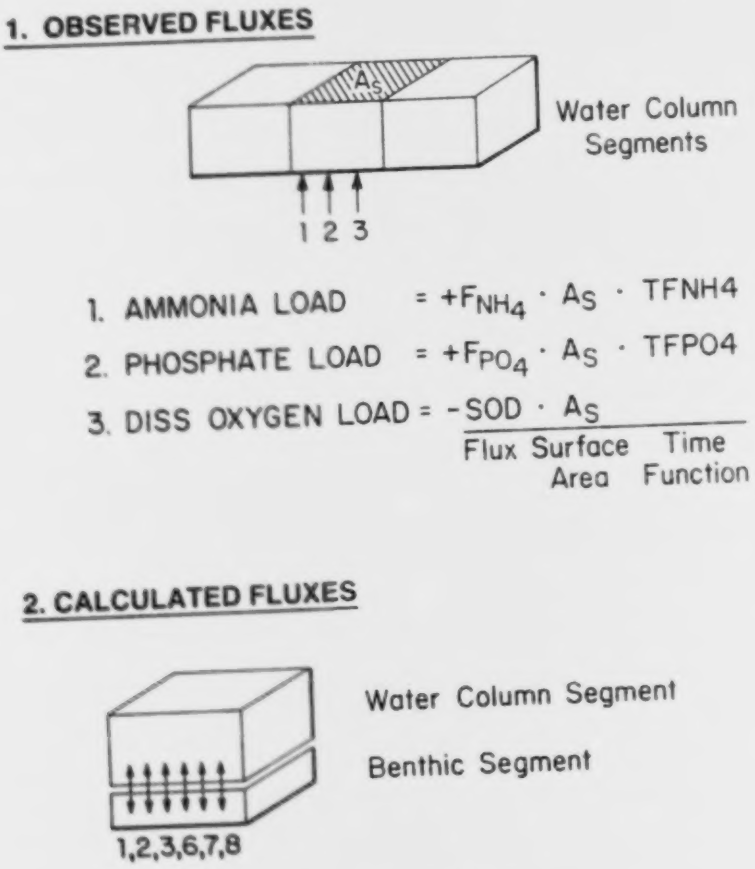

1. OBSERVED FLUXES
A_s
Water Column Segments
1 2 3
1. AMMONIA LOAD = $+F_{NH_4} \cdot A_S \cdot$ TFNH4
2. PHOSPHATE LOAD = $+F_{PO_4} \cdot A_S \cdot$ TFPO4
3. DISS OXYGEN LOAD = $-SOD \cdot A_S$
Flux
Surface Area
Time Function
2. CALCULATED FLUXES
Water Column Segment
Benthic Segment
1,2,3,6,7,8

Figure 30. Sediment-water exchange.

• The calculational framework incorporated for benthic-water column exchange draws principally from a study of Lake Erie, which incorporated sediment-water column interactions, performed by Di Toro and Connolly (1980). The mass-balance equations for dissolved and particulate materials are presented first, principally to show mass transport, followed by the descriptions of the kinetics for nitrogen, oxygen, and phosphorus as were incorporated in the modeling framework.

For a one-layer benthic layer with thickness, h, the particulate and dissolved mass balance equations are respectively:

$$\frac{\partial C_{pi}}{\partial t} = \frac{v_s}{h} \cdot C_{pj} - \frac{v_{sd}}{h} \cdot C_{pi} - k_p \cdot C_{pi} \qquad 95$$

and

$$\frac{\partial C_{wi}}{\partial t} = \frac{E}{h^2} \cdot (C_{wj} - C_{wi}) - \frac{v_{sd}}{h} \cdot C_{wi} - k_w \cdot C_{wi} \qquad 96$$

where:

$i, j,$ = indicates benthic layer and water column, respectively

C_{pi}, C_{pj} = the particulate material concentrations in the benthic layer and water column respectively, mg/l

C_{wi}, C_{wj} = the dissolved concentrations in the benthic interstitial waters and overlying water column respectively, mg/l

v_s = the net settling velocity of particulates across the water column-benthic interface, ft/day

v_{sd} = the sedimentation velocity induced by sedimentation, relative to a coordinate system fixed with respect to the benthic surface, ft/day

E = the diffusive exchange rate between dissolved concentrations in the interstitial water and the overlying water column, ft^2/day

k_p, k_w = first order reaction rates associated with the particulate and dissolved phases respectively, day^{-1}.

A more detailed parameterization of settling into the benthos would include not only a downward settling velocity but an upward resuspension velocity as well. In this context, then, the single settling velocity used in these computations can be thought of as the settling velocity that represents the net flux to the sediment due to the difference between the downward settling flux and the upward resuspension flux.

One of the first decisions to be made regarding the benthic layer is to determine its depth. Two factors influence this decision. The first is to adequately reflect the thickness of the active layer, the depth to which the sediment is influenced by exchange with the overlying water column. Secondly one wishes the model to reflect a reasonable time history or "memory" in the sediment layer. Too thin a layer and the benthos will "remember" or be influenced by deposition of material that would have occurred only within the last year or two of the period being analyzed; too thick a layer and the model will "average" too long a history, not reflecting, as in the case of phosphorus, substantial reductions in sedimentary phosphorus resulting from reduced phosphorus discharges from sewage treatment plants. The choice of sediment thickness is further complicated by spatially variable sedimentation rates. The benthic layer depths, together with the assigned sedimentation velocities, provide for a multi-year detention time or "memory', providing a reasonable approximation of the active layer in light of the observed pore water gradients.

The next consideration is the application of these mass balance equations to the nitrogen species in a reducing sediment (Berner, 1974). Particulate organic nitrogen is hydrolyzed to ammonia by bacterial action within the benthos. In addition to the ammonia produced by the hydrolysis of particulate organic nitrogen in the benthos, ammonia is generated by the anaerobic decomposition of algae. In a study of this reaction, Foree and McCarty (1970) showed that the anaerobic rate of decay of algae is substantial (0.007-0.022 day^{-1}). However, the end product initially is not exclusively ammonia. Rather, a fraction of the algal nitrogen becomes particulate organic nitrogen, which must undergo hydrolysis before becoming ammonia.

Ammonia produced by the hydrolysis of non-algal organic nitrogen and the decomposition of detrital algal nitrogen may then be exchanged with the overlying water column via diffusion. No nitrification occurs in the sediment due to the anaerobic conditions present in the sediment. Denitrification, the conversion of nitrate to nitrogen gas, may occur, however. Nitrate is present in the benthos due to diffusive exchange with the overlying water column.

The analysis of the benthic nitrogen concentrations and the resulting flux of ammonia is relatively straightforward because of the simplicity of the kinetics: hydrolysis and anaerobic algal decay produce a stable end product, ammonia, which does not undergo further reactions in the anaerobic sediment. The equations resulting from the above framework are presented in Table 9.

The reactions that convert algal and refractory carbon to their end products are more complex. The initial step in which the algal and refractory carbon are converted to reactive intermediates appears to be similar to the refractory organic and algal nitrogen degradation, and in the subsequent calculations, the rates for carbon and nitrogen decomposition are assumed to be equal. The reactive intermediates, however, participate in further reactions: for example, volatile acids react to become methane, and the mechanisms that control these reactions are somewhat uncertain. In addition, few measurements of these intermediate species are available and a calculation that incorporates their concentrations explicitly would of necessity be speculative. Thus, one uses a simplified, yet realistic, formulation of these reactions.

The method proposed by Di Toro and Connolly (1980), and highlighted here, is based upon separating the initial reactions that convert sedimentary organic material into reactive intermediates and the remaining redox reactions that occur. Then using a transformation variable and an orthogonality relationship, DiToro and Connolly derive mass balance equations that are independent

TABLE 9. SEDIMENT LAYER NITROGEN REACTION TERMS

Total Organic Nitrogen (TON)

$$S_{10j} = a_{NC} f_{ON} (k_{PZD} \theta_{PZD}{}^{T-20}) [P_c] - k_{OND} \theta_{OND}{}^{T-20} [TON]$$

Ammonia Nitrogen

$$S_{13j} = a_{NC} f_{NH_3} (k_{PZD} \theta_{PZD}{}^{T-20}) [P_c] + k_{OND} \theta_{OND}{}^{T-20} [TON]$$

Nitrate Nitrogen

$$S_{14j} = k_{140} \theta_{140}{}^{T-20}$$

Sediment Ammonia Flux Rate

$$NH_{3\,flux} = \frac{E_{DIF}}{h} \left([NH_3]_{sl} - [NH_3]_{wc} \right)$$

(positive rate + flux from sediment to water column)

Sediment Nitrate Flux Rate

$$NO_{3\,flux} = \frac{E_{DIF}}{h} \left([NO_3]_{sl} - [NO_3]_{wc} \right)$$

(negative rate + flux from water column into sediment)

TABLE 9. SEDIMENT LAYER NITROGEN REACTION TERMS (Continued)

Description	Notation	Value from Potomac Estuary Study	Units
Anaerobic algal decomposition rate	k_{PZD}	0.02	day^{-1}
Temperature coefficient	θ_{PZD}	1.08	none
Organic nitrogen decomposition rate	k_{OND}	0.0004	day^{-1}
Temperature coefficient	θ_{OND}	1.08	none
Diffusive exchange coefficient	E_{DIF}	2.0-2.5	cm^2/day
Benthic layer depth	h	0.22-0.67	ft
Benthic layer	bl		
Water column	wc		

of the details of the redox equations. Rather they are only functions of the component concentration, and it suffices to compute only the component concentrations, which can be treated in exactly the same way as any other variable in the mass transport calculation.

The convenient choice of components for the calculation are those that parallel the aqueous variables: carbonaceous BOD and dissolved oxygen. Restricting the calculation to these components, however, eliminates the possibility of explicitly including the effects of other reduced species such as iron, manganese, and sulfide, which play a role in overall redox reactions and may be involved in the generation of sediment oxygen demand. This simplication appears reasonable in light of the preliminary nature of the benthic calculation.

The decomposition reactions that drive the component mass balance equations are the anaerobic decomposition of the algal carbon, and the anaerobic breakdown of the benthic organic carbon. Both reactions are sinks of the oxygen and rapidly drive its concentration negative, indicating that the sediment is reduced rather than oxidized. The negative concentrations computed can be considered the oxygen equivalents of the reduced end products produced by the chains of redox reactions occurring in the sediment.

Because the calculated concentration of oxygen is positive in the overlying water, it is assumed that the reduced carbon species (negative oxygen equivalents) that are transported across the benthic water interface combine with the available oxygen and are oxidized to CO_2 and H_2O with a consequent reduction of oxygen in the overlying water column. The sediment mass balance equations for carbonaceous BOD and DO, together with the equation for sediment oxygen demand, are presented in Table 10.

TABLE 10. BENTHIC LAYER BOD_5 AND DO REACTION RATES

Carbonaceous 5-day Biochemical Oxygen Demand

$$S_{18j} = a_{OC}k_{PZD}\theta_{PZD}^{T-20}[P_C] - k_{DS}\theta_{DS}^{T-20}[CBOD] - \frac{5}{4}a_{ON}k_{140}\theta^{T-20}[NO_3]$$

Dissolved Oxygen

$$S_{19j} = -k_{DS}\theta_{DS}^{T-20}[CBOD]$$

Sediment Oxygen Demand

$$SOD = \frac{E_{DIF}}{h}([DO]_{wc} - [DO]_{bl})$$

(positive rate → flux from water column into benthos)

Description	Notation	Value	Units
Organic carbon (as CBOD) decomposition rate	k_{DS}	.0004	day^{-1}
Temperature coefficient	θ_{DS}	1.08	none
Diffusive exchange coefficient	E_{DIF}	cf. Table 9	
Benthic layer depth	h		
Benthic layer	bl		
Water Column	wc		

A complete analysis of the phosphorus fluxes from sediments would require a rather complex and elaborate computation of solute-precipitate chemistry and its interaction with the mass transport of the dissolved species. The reasons for this are twofold: first, it is well known (Nriagu, 1972) that for phosphorus the formation of precipitates affects the interstitial water concentrations, thereby affecting the interstitial water transport of the various phsophorus forms or species; second, the dissolved concentrations are affected by the redox reactions, which in turn, affect the phosphorus fluxes that occur during aerobic and anaerobic conditions. (Phosphorus fluxes are enhanced under anaerobic conditions).

A computation of solute-precipitate chemistry was judged to be outside the scope of this study. Instead, a simplified approach was taken, which to a large degree relies on empiricism. Anaerobic decomposition of refractory organic phosphorus and detrital algal phosphorus is assumed to occur using the same rate expressions and rate constants as those for organic nitrogen. However, the fraction of the end product, dissolved inorganic phosphorus, that remains in the interstitial water is not involved in the formation of precipitates or being sorbed onto the benthic solids but varies spatially. This spatial variation reflects of the ionic chemical make up of the benthos in various regions of the water body.

Using observed total and interstitial dissolved inorganic phosphorus values, the fraction particulate (or sorbed) inorganic phosphorus can be assigned as a segment parameter, with the particulate and dissolved inorganic phosphorus computed for each time step in a manner similar to the overlying water column inorganic phosphorus (equations 79 through 81). Exchange of the dissolved phosphorus forms with the overlying water column is also similar to that of ammonia, nitrate, and dissolved oxygen. Mass balance equations are presented in Table 11. The effects of anoxia upon sediment phosphorus flux were not included in the modeling framework. The approach used to generate sediment phosphorus flux, although not entirely satisfactory, is at least consistent with the framework within which the fluxes of other materials are being generated.

1.5 THE TOXIC CHEMICAL MODEL

TOXIWASP is a dynamic compartment model of the transport and fate of organic chemicals and metals in all types of aquatic systems. It combines the hydrodynamic capabilities discussed in Section 1.2 and the transport capabilities discussed in Section 1.3 with the sediment balance and chemical transformation capabilities discussed here. The chemical transformations were adopted from EXAMS (Burns et al., 1982), which remains a good reference manual.

1.5.1 Overview of TOXIWASP

Several physical-chemical processes can affect the transport and fate of toxic chemicals in the aquatic environment. The most important are pictured in Figure 31, taken from the chapter on aquatic chemistry in Mills et al. (1985). TOXIWASP explicitly handles most of these, excluding only acid-base equilibria, reduction, and precipitation-dissolution.

TOXIWASP simulates the transport and transformation of a single chemical and total sediment in water column and benthic segments. Within each segment the chemical is divided into three phases: dissolved, sorbed, and biosorbed, as illustrated in Figure 32. Because local equilibrium among the phases is assumed, they constitute a single state variable, or WASP system. TOXIWASP, then, is composed of two systems, chemical and sediment, for which the general WASP3 mass balance equation is solved:

TABLE 11. BENTHIC LAYER PHOSPHORUS REACTION TERMS

Dissolved Organic Phosphorus (DOP)

$$S_{5j} = a_{PC} f_{DOP} (k_{PZD} \theta_{PZD}^{T-20}) [P_c] - k_{OPD} \theta_{OPD}^{T-20} [DOP]$$

Particulate Organic Phosphrous (POP)

$$S_{6j} = a_{PC} f_{POP} (k_{PZD} \theta_{PZD}^{T-20}) [P_c] - k_{OPD} \theta_{OPD}^{T-20} [POP]$$

Dissolved Inorganic Phosphorus (DIP)

$$S_{8j} = a_{PC} f_{DIP} (k_{PZD} \theta_{PZD}^{T-20}) [P_c] - k_{OPD} \theta_{OPD}^{T-20} ([DIP]+[POP])$$

Particulate Inorganic Phosphorus (PIP)

$$S_{9j} = 0$$

State Equations

Total Inorganic Phosphorus (TIP)

$$TIP = DIP + PIP$$

$$PIP = f_{Pbl} \cdot TIP$$

$$DIP = (1 - f_{Pbl}) \cdot TIP$$

Sediment Phosphorus Flux Rate

$$P_{flux} = \frac{E_{DIF}}{h} \left\{ ([DIP]_{bl} - [DIP]_{wc}) + ([DOP]_{bl} - [DOP]_{wc}) \right\}$$

(positive rate → flux from sediment to water column)

TABLE 11. BENTHIC LAYER PHOSPHORUS REACTION TERMS (Continued)

Description	Notation	Value	Units
Organic phosphorus decomposition rate	k_{OPD}	0.0004	day^{-1}
Temperature coefficient	θ_{OPD}	1.08	none
Fraction particulate in the sediment layer	f_{pbl}	0.955- 0.999	none
Diffusive exchange coefficient	E_{DIF}	cf. Table 9	
Benthic layer depth	h		
Benthic layer	bl		
Water Column	wc		

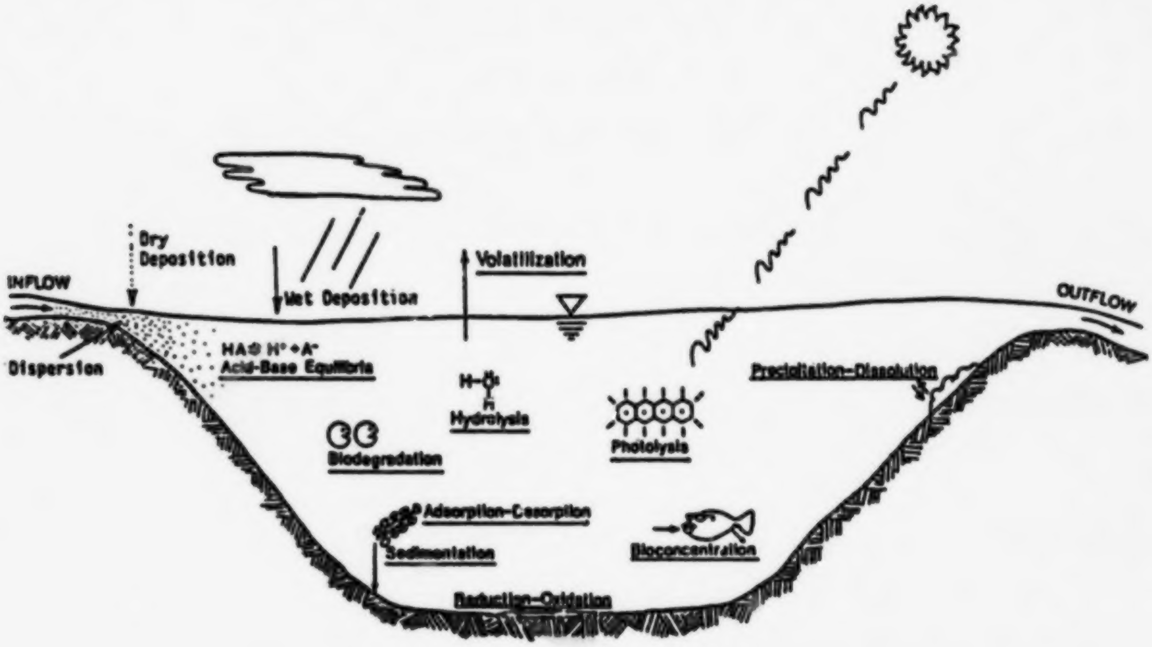

Dry Deposition
Wet Deposition
Volatilization
INFLOW
OUTFLOW
Dispersion
HA ⇌ H⁺ + A⁻
Acid-Base Equilibria
Hydrolysis
Photolysis
Precipitation-Dissolution
Biodegradation
Adsorption-Desorption
Sedimentation
Bioconcentration
Reduction-Oxidation

Figure 31. Speciation, transport and transformation processes in the aquatic environment (Mill et al. 1985).

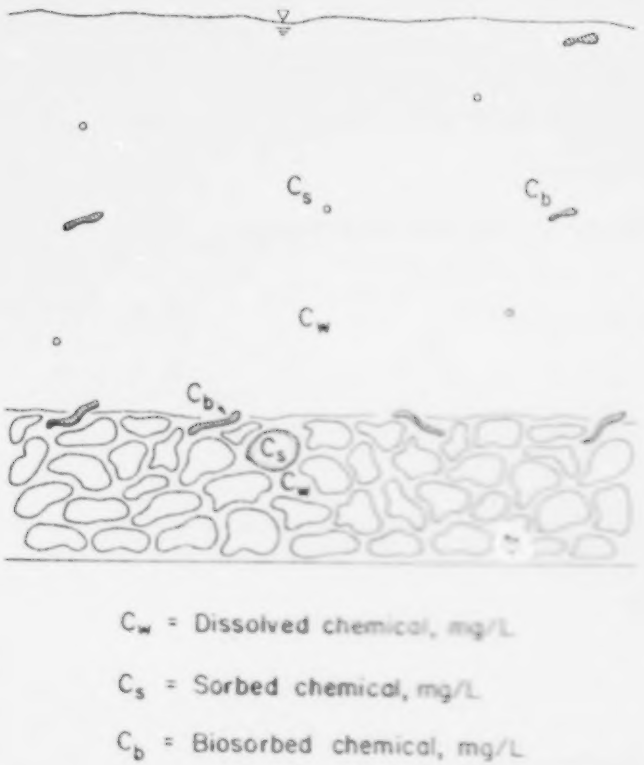

C_s
C_b
C_w
C_b
C_s
C_w
C_w = Dissolved chemical, mg/L
C_s = Sorbed chemical, mg/L
C_b = Biosorbed chemical, mg/L

Figure 32. Physical-chemical processes.

$$\frac{\Delta (V_j \cdot C_j)}{\Delta t} = \sum_i [-Q_{ij} \cdot C_{ij} + R_{ij} \cdot (C_i - C_j)] + \sum_L W_{Lj} + \sum_B W_{Bj} + \sum_k V_j \cdot S_{kj} \qquad 97$$

where:

V_j = volume of segment j, L^3

C_j = concentration of the water quality constituent in segment j, M/L^3

t = time, T

Q_{ij} = advective flow between segments i and j, defined as positive when leaving segment j, and negative when entering, L^3/T

C_{ij} = constituent concentration advected between i and j, M/L^3

= $\nu \cdot C_j + (1 - \nu) \cdot C_i$ when entering j

= $\nu \cdot C_i + (1 - \nu) \cdot C_j$ when leaving j

ν = numerical weighting factor, 0-0.5

R_{ij} = dispersive flow between segments i and j, L^3/T

$$= \frac{E_{ij} \cdot A_{ij}}{\ell_{ij}}$$

E_{ij} = dispersion coefficient between segments i and j, L^2/T

A_{ij} = cross-sectional area between segments i and j, L^2

ℓ_{ij} = characteristic mixing length betwen segments i and j, L

W_{Lj} = point and diffuse loads into segment j, M/T

W_{Bj} = boundary loads into segment j, M/T

S_{Kj} = kinetic transformations within segment j, $M/L^{-3}/T$

To this general equation, the TOXIWASP subroutines add specific transport processes, including settling, deposition, scour, sedimentation, pore water percolation, pore water diffusion, and benthic-water column dispersive exchange. The net effect is to customize equation 97 for the four general cases of chemical and sediment in water column and benthos:

Sediment in Water Column--

$$\frac{\Delta (V_j \cdot S_j)}{\Delta t} = \sum_i [-Q_{ij} \cdot S_{ij} - w_{sij} \cdot A_{ij} \cdot S_j + R_{ij} \cdot \Delta S_{ij}] + \sum_L W_{Ls} + \sum_B W_{Bjs} \qquad 98$$

Chemical in Water Column--

$$\frac{\Delta (V_j \cdot C_j)}{\Delta t} = \sum_i [-Q_{ij} \cdot C_{ij} - w_{sij} \cdot A_{ij} \cdot S_j \cdot C'_{sj} + R_{ij} \cdot \Delta C_{ij}]$$

$$+ \sum_L W_{Ljc} + \sum_B W_{Bjc} + \sum_k V_j \cdot S_{kjc} \qquad 99$$

Sediment in Bed--

$$\frac{\Delta\,(V_j \;.\; S_j)}{\Delta t} = \sum_i \left[-W_{sed,ij} \cdot A_{ij} \cdot S_j\right] - \sum_B W_{Bjs} = 0 \qquad 100$$

Chemical in Bed--

$$\frac{\Delta\,(V_j \;.\; C_j)}{\Delta t} = \sum_i \left[-Q_{ij} \cdot C'_{wij} - w_{sedij} \cdot A_{ij} \cdot C_j + Q_{pj} \cdot C'_{wj} + R_{Bij}\;\Delta\;C'_{wij}\right]$$

$$+ \sum_L W_{Ljc} - \sum_B W_{Bjc} + \sum_k V_j \cdot S_{kjc} \qquad 101$$

where:

C = chemical concentration, M/L^3

C'_w = dissolved chemical concentration, M/L^3_{water}

C'_s = sorbed chemical concentration, $M/M_{sediment}$

S = sediment concentration, M/L^3

w_{sij} = settling velocity in water, positive leaving j, negative entering j, L/T

w_{sedij} = sediment velocity in bed, positive leaving j, negative entering j, L/T

Q_{pj} = pore water flow generated by sediment compaction, L^3/T

R_{Bij} = pore water diffusive exchange flow, L^3T^{-1}

$$= \frac{E_{ij} \cdot A_{ij}}{\ell_{ij}} \cdot \frac{n_{ij}}{t_{ij}} \qquad 102$$

t_{ij} = average tortuosity of segments i and j, L_{water}/L

n_{ij} = average porosity of segments i and j, L^3_{water}/L^3

subscript c = refers to chemical

subscript s = refers to sediment

The processes of deposition, scour, and benthic-water column dispersive exchange are considered special boundary loads expressed in the term $\sum_B W_{Bj}$. Their functional forms are developed below.

In addition to these transport processes, the TOXIWASP subroutines add specific chemical transformation processes. From chemical characteristics of a compound and the environmental parameters of the system, TOXIWASP formulates a total transformation rate. This rate is based on a simple addition of the pseudo-first order rates for hydrolysis, photolysis, oxidation, and biodegradation. In addition, the volatilization rate is calculated and added to the transformation rate. Sorption onto sediment and onto biomass is calculated assuming local equilibrium, using a chemical-specific partition coefficient and spatially varying environmental organic carbon fractions. These transformation processes are expressed in the term $\sum_k S_{kj}$. Their functional forms are developed below.

TOXIWASP uses equations 98 - 101 to calculate sediment and chemical mass and concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed. Three examples are given in Figure 33. In a simulation, sediment is treated as a conservative constituent that is advected and dispersed among water segments, that settles to and erodes from benthic through net sedimentation or erosion. Benthic sediment concentrations remain constant, with the upper benthic volume expanding or contracting to conserve mass.

In a simulation, the chemical undergoes first-order decay, based on summation of several process rates, some of which are second-order. Thus, the effective first order decay rate can vary with time, and space, and is recalculated as often as necessary throughout a simulation. The chemical is advected and dispersed among water segments, and exchanged with surficial benthic segments by dispersive mixing. Sorbed chemical settles through water column segments and deposits to or erodes from surficial benthic segments. Within the bed, dissolved chemical migrates downward or upward through percolation and pore water diffusion. Sorbed chemical migrates downward or upward through net sedimentation or erosion. No lateral migration of the chemical within the bed is allowed.

Some limitations should be kept in mind when applying TOXIWASP. First, chemical concentrations should be near trace levels, i.e., below half the solubility or 10^{-5} molar. At higher concentrations, the assumptions of linear partitioning and transformation begin to break down. Chemical density may become important, particularly near the source, such as in a spill. Large concentrations can affect key environmental characteristics, such as pH or bacterial populations, thus altering transformation rates. TOXIWASP does not include such feedback phenomena.

It should be noted that TOXIWASP, like WASP3, requires the user to specify the flow field. Flows can be based on measurements, simple continuity calculations, or on hydrodynamic model simulations. WASP3 does not check the flow field for inconsistencies, which may lead to mass balance errors. The user should take care to check the specified flows for errors. For simulations using hydrodynamic results from DYNHYD3, volumes and flows

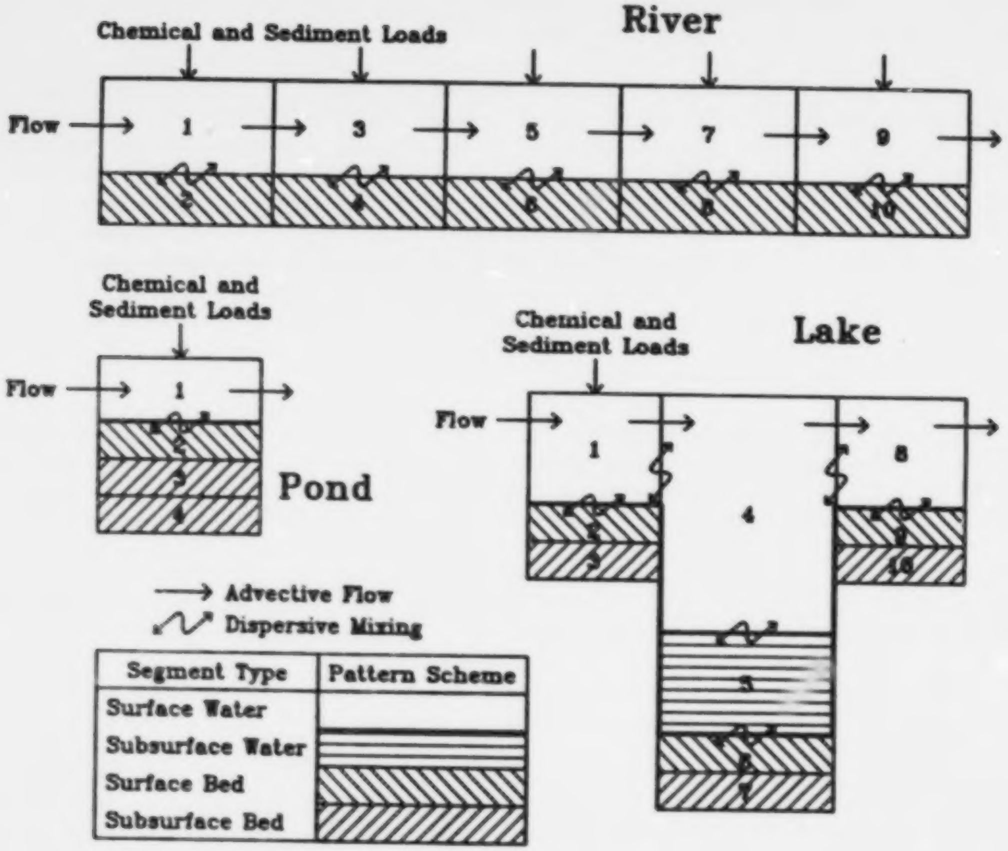

River
Chemical and Sediment Loads
Flow
1
2
3
4
5
6
7
8
9
10
Chemical and Sediment Loads
Flow
1
2
3
4
Pond
Chemical and Sediment Loads
Lake
Flow
1
2
3
4
5
6
7
8
9
10
Advective Flow
Dispersive Mixing
Segment Type
Pattern Scheme
Surface Water
Subsurface Water
Surface Bed
Subsurface Bed

Figure 33. Examples of TOXIWASP network configuration.

from the SUMRY2 file are used directly, and flow continuity is maintained.

In the following development it is convenient to define concentration related symbols as in Table 12.

1.5.2 The Sediment System

Sediment transport is potentially a very important process influencing chemical transport and fate. Many chemicals sorb strongly to sediment and thus undergo settling, scour, and sedimentation. Sorption also affects a chemical's transfer and transformation rates. Volatilization and base-catalyzed hydrolysis, for example, are slowed by sorption. Both sediment transport rates and concentrations must be estimated in most toxic chemical studies.

TABLE 12. CONCENTRATION RELATED SYMBOLS USED IN MATHEMATICAL EQUATIONS

Symbol	Definition	Units
C_j	Concentration of total chemical in segment j.	mgc/L
C_{wj}	Concentration of dissolved chemical in segment j.	mgc/L
C'_{wj}	Concentration of dissolved chemical in water in segment j. $C'_{wj} = C_{wj}/n_j$	mgc/L_w
C_{sj}	Concentration of sorbed chemical in segment j.	mgc/L
C'_{sj}	Concentration of sorbed chemical on sediment in segment j. $C'_{sj} = C_{sj}/S_j$	mgc/kgs
C_{bj}	Concentration of biosorbed chemical in segment j.	mgc/L
C'_{bj}	Concentration of biosorbed chemical in biota in segment j. $C'_{bj} = C_{bj}/B_j$	mgc/kgb
s_j	Concentration of sediment in segment j.	mgs/L
S_j	Concentration of sediment in segment j. $S_j = s_j \cdot 10^{-6}$	kgs/L
S'_j	Concentration of sediment in water in segment j $S'_j = S_j/n_j$	kgs/L_w
B_j	Concentration of biomass in segment j.	kgb/L
B'_j	Concentration of biomass in water in segment j $B'_j = B_j/n_j$	kgb/L_w
n_j	Porosity or volume water per volume segment j.	L_w/L
K_{ps}	Partition coefficient of chemical on sediment in segment j.	L_w/kgs
K_{pB}	Partition coeffiient of chemical on biomass.	L_w/kgb

Investigators (Karickhoff et al., 1979; Rao and Davidson, 1980) have shown that for most organic toxicants, particularly non-polar compounds, the sediment organic matter determines the extent of sorption and hence the importance of sorbed-pollutant transport. The particle size of the sediments is influential, but Rao and Davidson (1980) have shown that the organic matter content of each size fraction is the controlling factor. Organic matter content and surface area relationships suggest that silt and clay-size sediment fractions are most relevant in sediment transport.

One outcome of this rationale is the idea that, in river systems, wash load or suspended sediment is the important pollutant transport medium rather than bed load. If bed load transport can be ignored, the problem remains to estimate suspended sediment. In general, the stream transport capacity for wash load is in excess of its actual load, and the problem is one of estimating sediment source loading--namely, watershed erosion. In areas of backwater behind dams or in sluggish reaches, the stream transport capacity may drop enough to allow net deposition. Strongly sorbed pollutants may build up significantly. Because sediment transport can be complex, sitespecific calibration of the settling, scour, and sedimentation rates is usually necessary.

TOXIWASP treats sediment in the water column and the bed as a conservative substance governed by equations 98 and 100. The major processes of advective and dispersive transport, sediment loading, benthic exchange, and bed sedimentation and erosion are presented in the following sections. An overview of TOXIWASP sediment processes is given in Figure 34.

1.5.2.1 Suspended Sediment Transport

Advective and dispersive flows carry suspended sediment to adjacent water segments. Standard WASP input for flows, dispersion coefficients, cross-sectional areas, and characteristic lengths must be specified. In addition, TOXIWASP allows settling to lower water segments and deposition to surficial bed segments. Settling velocities w_s should be set within the range of Stoke's velocities corresponding to the suspended particle size distribution:

$$V_s = \frac{8.64 \cdot g}{18 \cdot \mu} \cdot (\rho_p - \rho_w) \cdot d_p^2 \qquad 103$$

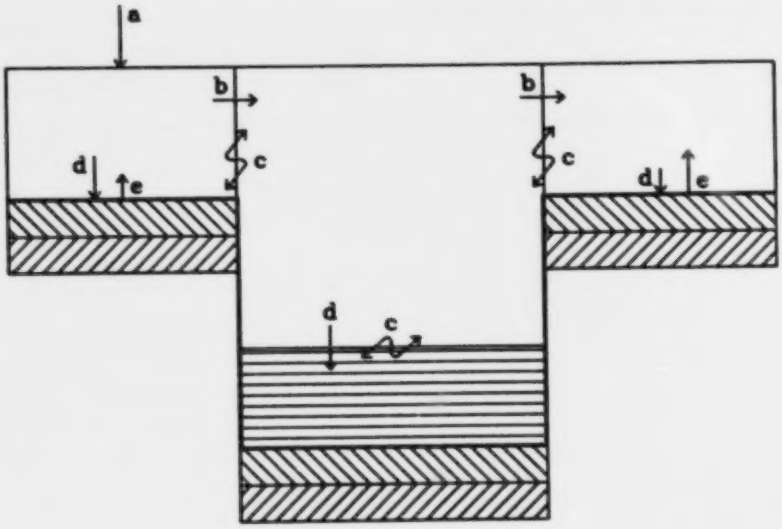
where:

V_s = Stokes velocity for particle with diameter d_p and density ρ_p, m/day

g = acceleration of gravity = 981 cm/sec^2

μ = absolute viscosity of water = 0.01 poise (g/cm^2-sec) at 20°C

d_p = particle diameter, mm



Process	**Segment Types**
a) Mass Loading	**1,2 to Water**
b) Advection	**1,2 Water–Water**
c) Dispersion	**1,2 Water–Water**
d) Settling	**1,2 Water–Water or Water–Bed**
e) Erosion	**3 Surface Bed–Water**

Figure 34. TOXIWASP sediment transport processes.

Values of V_s for a range of particle sizes and densities are provided in Table 13. Deposition velocities should be set to some fraction of V_s, as discussed in the section on benthic exchange. Spatially variable settling velocities can be specified using parameter WS(ISEG) for appropriate water column segments.

1.5.2.2. Sediment Loading

Sediment loading derives primarily from watershed erosion and bank erosion. These can be measured or estimated by several techniques, and input into each segment as a waste load. For some problems, long term average sediment loads can be calculated using the Universal Soil Loss Equation (Wischmeier and Smith, 1965). A useful treatment of this process is given

TABLE 13. STOKE'S SETTLING VELOCITIES AT 20°C

Particle Diameter, mm	Particle Density, g/cm^3 1.8	2.0	2.5	2.7
Fine Sand				
0.2	380	470	710	800
0.05	94	120	180	200
Silt				
0.05	94	120	180	200
0.02	15	19	28	32
0.01	3.8	4.7	7.1	8.0
0.005	0.94	1.2	1.8	2.0
0.002	0.15	0.19	0.28	0.32
Clay				
0.002	0.15	0.19	0.28	0.32
0.001	0.04	0.05	0.07	0.08

Settling velocities in m/day

by Mills et al. (1985). This technique works poorly for short term or inherently dynamic problems because much of the sediment loading occurs during a few extreme storm or snow melt events. If available, suspended sediment data at local gaging stations can be extrapolated to provide area-wide loading estimates. Alternatively, daily runoff loads can be simulated with a watershed model and read-in directly from an appropriately formatted nonpoint source loading file.

1.5.2.3. Benthic Exchange

Benthic exchange of sediment is driven by the net scour and deposition velocities:

$$W_{Bs} = A_{ij} \cdot (w_R \cdot S_i - w_D \cdot S_j) \qquad 104$$

where:

w_R = scour velocity, L/T

w_D = deposition velocity, L/T

A_{ij} = benthic surface area, L^2

i = benthic segment

j = water segment

The deposition velocity can be calculated as the product of the Stokes settling velocity and the probability of deposition:

$$w_D = w_s \cdot \alpha_D \qquad 105$$

where:

α_D = probability of deposition upon contact with the bed.

The probability of deposition depends upon the shear stress on the benthic surface and the suspended sediment size and cohesiveness. Likewise, the scour velocity depends upon the shear stress, the bed sediment size and cohesiveness , and the state of consolidation of surficial benthic deposits. Figure 35 is offered as initial guidance in specifiying initial deposition and scour velocities. For example, course silt of 0.05 mm diameter may settle at 100 to 200 m/day, but should not deposit where mean stream velocity is above 0.5 cm/sec. Where mean velocity rises above 30 cm/sec, erosion is expected, and nonzero scour velocities should be specified. For fine silt of 0.005 mm diameter settling at 1 to 2 m/day, deposition is not expected, even under quiescent conditions. Nonzero scour velocities should be specified where mean velocity is above 2 m/sec. Site-specific calibration is necessary to refine the initial estimates. Spatially variable deposition and scour velocities are read-in using the parameter WS(ISEG). These are net, time-averaged velocities. If time-variable deposition and scour velocities are necessary, guidance is available for altering the program appropriately.

1.5.2.4 Bed Sedimentation and Erosion

TOXIWASP treats bed sediment as a conservative substance that migrates down or up with respect to the bed surface in response to net sedimentation or erosion. The governing equation 100 presented above is written with respect to the bed surface and has two terms in equilibrium-sedimentation and benthic exchange. When sediment deposition exceeds sediment scour, W_{Bs} is negative and net deposition leads to a rising bed surface and burial of sediment and sorbed chemical. When sediment scour exceeds sediment deposition, W_{Bs} is positive and net erosion leads to a falling bed surface and release of previously buried sediment and sorbed chemical.

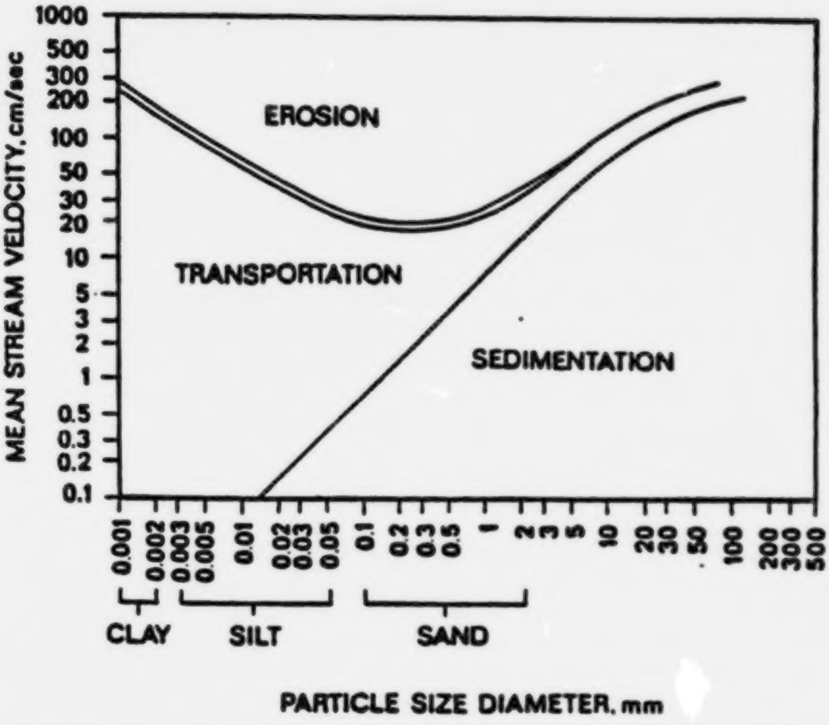


Figure 35. Relationship between stream velocity, particle size, and the regimes of sediment, erosion, transport, and deposition (Graf 1971).

A simple method for treating sedimentation is to define bed segment locations in reference to the rising or falling bed surface. If the bed surface rises at w_{sed} cm per year, then buried sediment and chemical descend through the bed at w_{sed} cm per year in reference to the rising bed segments (all other bed dispersion processes being ignored for the moment). There are two complications in this approach. First, if the density of the bed increases with depth, then compression must be occurring, decreasing w_{sed} and squeezing the pore water and dissolved chemical upward. Second, the simulation time step is extemely short in relation to the net sedimentation velocity. This leads to rather severe "numerical dispersion," a form of computational inaccuracy within the bed.

To handle the first complication, TOXIWASP assumes two types of bed sediment: an upper uncompacted layer with sediment concentration S_j and lower, compacted layers with sediment concentration S_i. Given the assumption of sedimentation in equilibrium with net deposition, all physical bed properties remain constant. When sediment mass W_{Bs} is added to the upper layer, the same mass is transferred to lower layers. The sediment volume added to the upper layer is W_{Bs}/S_j, while the volume added to the lower layer is W_{Bs}/S_i. The difference in volumes is equal to the pore water volume squeezed out through compaction:

$$Q_{ps} = W_{Bs} \cdot (S_j^{-1} - S_i^{-1}) \qquad 106$$

where:

Q_{ps} = pore water flow from compaction, L^3/T

The rise in the bed surface equals the volume added to the lower layer divided by the surface area:

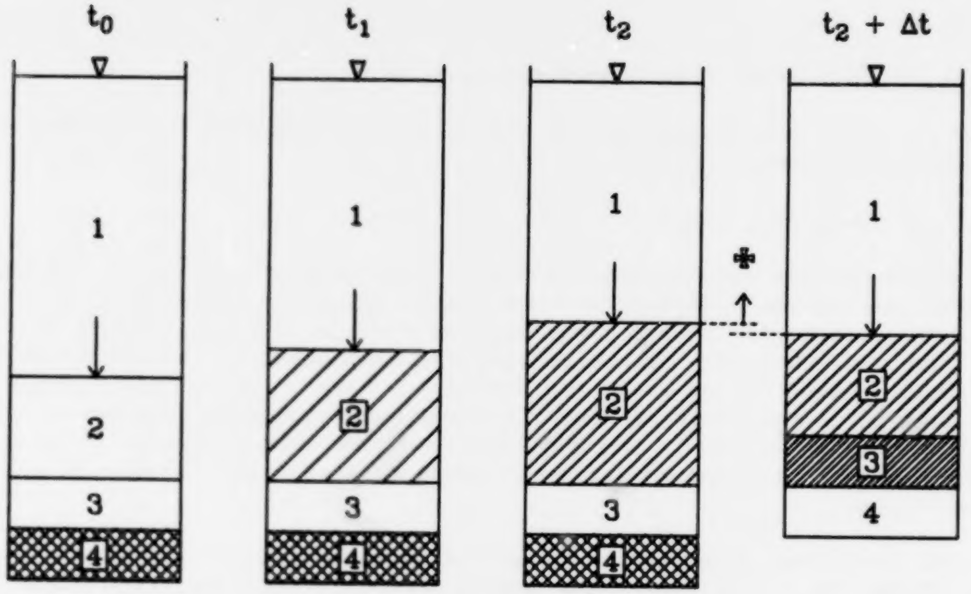
$$w_{sed} = W_{Bs}/(A_{ij} \cdot S_i) \qquad 107$$

To handle the second complication of numerical dispersion in the bed, TOXIWASP implements a version of this simple approach that amounts to a Lagrangian scheme for treating movement of chemical through the bed as a result of sedimentation. The time step for sedimentation is calculated internally, based on the scour and deposition rates. Whereas the simulation time step is on the order of hours, the sedimentation time step is on the order of months to years. The sedimentation time step varies with location and time and is tailored to minimize numerical dispersion in sedimentation calculations.

For locations where sediment deposition exceeds scour, TOXIWASP responds as in Figure 36. As sediment and sorbed chemical settle from the water column (segment 1) , the top bed segment (number 2) increases in volume, depth, chemical mass, and sediment mass. Its density remains constant. When the sediment mass in the top bed segment equals the initial sediment mass in the top two bed segments, then sediment compression is triggered. At this time the top bed segment depth (and volume) exceeds the initial top two bed segment depths (and volumes) as indicated in Figure 36. The top bed segment is now compressed into two segments.

The new top bed segment has the same depth, volume, and sediment mass as the initial top bed segment. The new second bed segment has the same depth, volume, and sediment mass as the initial second bed segment. (In fact, these properties of lower bed segments always remain constant.) The combined volume of the top two bed segments is now slightly less than the volume of the top bed segment just before compression. This volume represents pore water squeezed into the water column during compression. Chemical mass in the top two bed segments equals the chemical mass in the top bed segment just before compression minus the dissolved chemical mass in the pore water squeezed into the water column. Whereas chemical concentration remains constant in the top bed segment during the compression step, concentration increases in the new second bed segment where compression actually occurs.

Although this sedimentation algorithm minimizes numerical dispersion, it does lead to discontinuous concentration histories in lower bed segments as their locations are redefined. For "smoother" output with slightly higher numerical dispersion, TOXIWASP can recalculate sedimentation ten times per sedimentation time step. The user can adjust this ratio by altering the



	Time = t_0			Time = t_2			Time = $t_2 + \Delta t$		
Segment	**Depth**	**Density**	**Conc**	**Depth**	**Density**	**Conc**	**Depth**	**Density**	**Conc**
1	d_1	1.0	$C_1(0)$	$d_1 - d_2(2)$	1.0	$C_1(2)$	$d_1 - d_3$	1.0	$C_1(2)$
2	d_2	ρ_2	0.0	$d_2(0) + d_3\frac{\rho_3}{\rho_2}$	ρ_2	$C_2(2)$	d_2	ρ_2	$C_2(2)$
3	d_3	ρ_3	0.0	d_3	ρ_3	0.0	d_3	ρ_3	$C_2(2)\frac{\rho_3}{\rho_2}$
4	d_3	ρ_3	$C_4(0)$	d_3	ρ_3	$C_4(0)$	d_3	ρ_3	0.0

✚ Compaction: $\text{SVOL Compacted} = \text{Vol}(3)\left[\frac{\rho_3}{\rho_2} - 1\right]$

Pore water volume SVOL squeezed
into water column.

Figure 36. TOXIWASP sediment burial.

value of "FAC" (Constant 53) from 0.1.

The compression step does not affect any of the properties of the lower bed segments. In fact, even chemical concentration is unaffected at the third bed segment and below. Immediately following compression, however, TOXIWASP renumbers the lower bed segments, dropping the old bottom segment from the simulation. Chemical layers, then, are transferred downward intact and finally lost through the bottom. The accumulated mass lost through the bottom is saved and printed as variable BMASS(J), where "J" is the number of the bottom segment. Compression and renumbering completes the TOXIWASP sedimentation cycle (or time step).

For locations where sediment scour exceeds deposition, TOXIWASP responds as in Figure 37. As sediment and sorbed chemical erode from the bed, the top bed segment (number 2) decreases in volume, depth, chemical mass, and sediment mass. Its density remains constant. When the sediment mass in the top bed layer equals zero, then segment renumbering is triggered. All the properties of the remaining bed segments, including chemical concentration, remain unaffected by renumbering. The new top bed segment, for example, has the same depth, volume, sediment and chemical concentration as the old second bed segment. A new bottom bed segment is created with the same physical properties as the other bed segments. Its chemical concentration, however, is zero. Renumbering and creation of a new bottom segment completes the TOXIWASP erosion cycle (or time step).

As a consequence of the way TOXIWASP treats sedimentation, certain constraints are imposed on the bed segment properties defined in the input data set. The density (or sediment concentration) of a top bed segment (TYPEE = 3) must be greater than or equal to the density of the lower bed segments (TYPEE = 4) within a vertical stack. The volumes, depths, and densities of lower bed segments must be constant within a vertical stack. If a smooth representation of burial is desired, the volumes and depths of lower bed segments should be significantly smaller than the top bed layer.

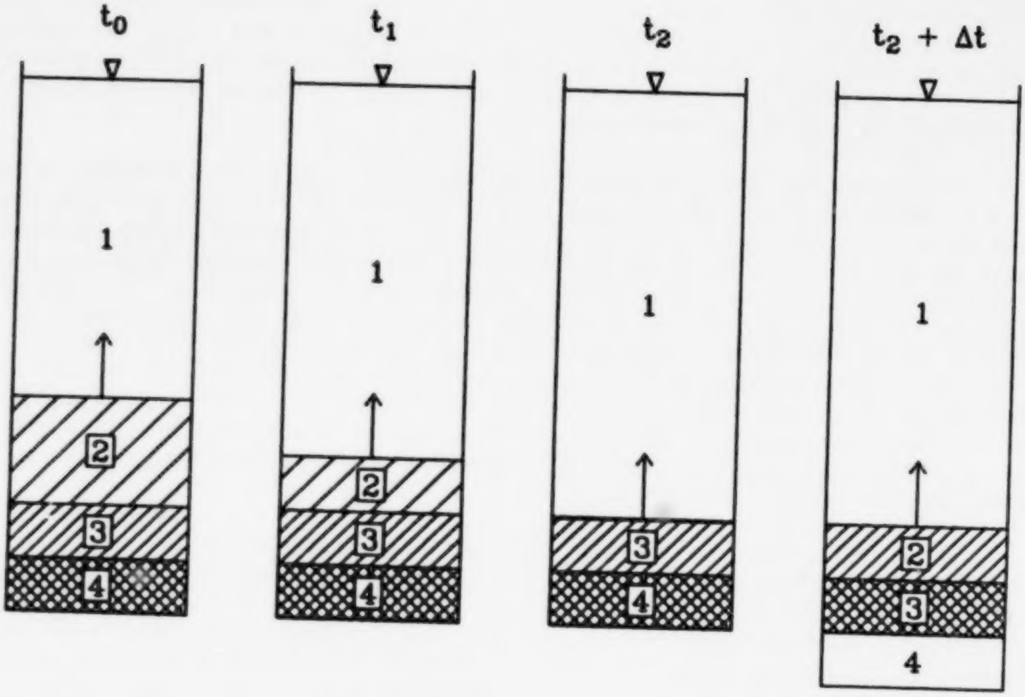
If lower bed segments are not included in a TOXIWASP network, then chemical burial will not take place. The upper bed layer will increase in volume and depth with settling, or decrease in volume and depth with scour. TOXIWASP prevents both complete filling of the water column and complete erosion of the bed.

Because sedimentation rates are calculated internally, the user need only specify initial conditions in the bed. TOXIWASP reads two parameters: initial sediment concentrations and the ratio of fresh (or wet) weight to dry weight (sometimes called "percent water"). If bulk densities are measured, sediment concentrations are given by

$$S = \rho_B - \rho_W \cdot n = \rho_B - n \qquad 108$$

where:

ρ_B = bulk density, kg (sediment and water)/L


t_0
t_1
t_2
$t_2 + \Delta t$
1
2
3
4
1
2
3
4
1
3
4
1
2
3
4

	Time = t_0			Time = t_2			Time = $t_2 + \Delta t$		
Segment	**Depth**	**Density**	**Conc**	**Depth**	**Density**	**Conc**	**Depth**	**Density**	**Conc**
1	d_1	1.0	0.0	$d_1+d_2(0)$	1.0	$C_1(2)$	$d_1+d_2(0)$	1.0	$C_1(2)$
2	d_2	ρ_2	$C_2(0)$	0	ρ_2	$C_2(0)$	d_3	ρ_3	$C_3(2)$
3	d_3	ρ_3	$C_3(0)$	d_3	ρ_3	$C_3(0)$	d_3	ρ_3	$C_4(2)$
4	d_3	ρ_3	$C_4(0)$	d_3	ρ_3	$C_4(0)$	d_3	ρ_3	0.0

Figure 37. TOXIWASP sediment erosion.

ρ_w = water density ≈ 1 kg (water)/L_w

Porosities can be derived from percent water by

$$n = \frac{(P-1)\frac{\rho_s}{\rho_w}}{1 + (P-1)\frac{\rho_s}{\rho_w}} \qquad 109$$

where:

ρ_s = sediment density ≈ 2.7, kg/L_s

P = percent water, or ratio of wet weight to dry weight, kg (sediment + water)/kg (sediment)

1.5.3 The Chemical System

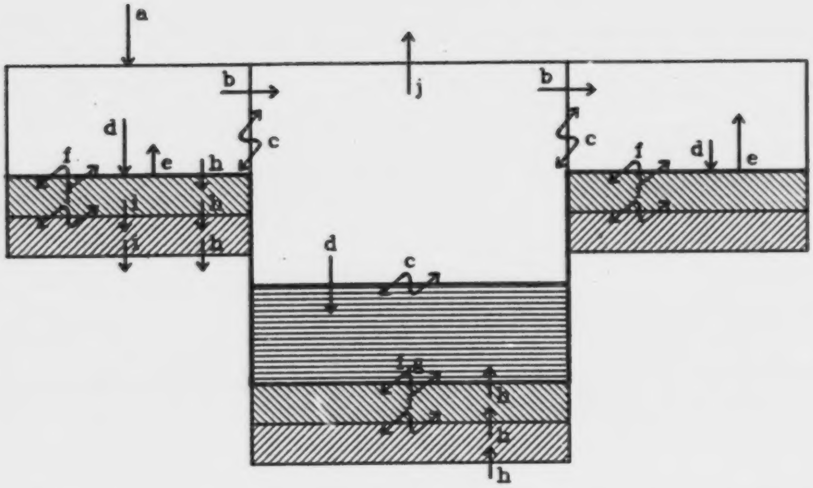
A compound transported through a water body can undergo several physical or chemical transformations. It is convenient to group these into fast and slow reactions. Fast reactions have characteristic reaction times on the same order as the model time step and are handled with the assumption of local equilibrium. Slow reactions have characteristic reaction times much longer than the model time step. These are handled with the assumption of local first order kinetics using a lumped rate constant specified by the user or calculated internally. Both rate constants and equilibrium coefficients must be estimated in most toxic chemical studies. Although these can be calculated internally from chemical properties and local environmental characteristics, site-specific calibration or testing is desirable.

TOXIWASP treats chemical in the water column and the bed as a reactive substance governed by equations 99 and 101. The major processes of advective and dispersive transport, chemical loading, benthic exchange, equilibrium sorption, kinetic transformation, and bed sedimentation and erosion are presented in the following sections. An overview of the TOXIWASP chemical transport and redistribution processes is given in Figure 38.

1.5.3.1 Advective and Dispersive Transport

Advective and dispersive flows carry chemical to adjacent water segments. Standard WASP input for flows, dispersion coefficients, cross-sectional areas, and characteristic lengths must be specified. In addition, TOXIWASP allows settling of sorbed chemical to lower water segments at the Stokes velocity w_s. Spatially variable settling velocities can be specified using parameter WS(ISEG) for appropriate water column segments.

Advective and dispersive flows between vertically adjacent benthic segments carry the dissolved chemical concentration C_{wij}. Advective flows can be specified using parameter WS(ISEG) for appropriate subsurface benthic



Process	Segment Types
a) Mass Loading	1,2 to Water
b) Advection	1,2 Water-Water
c) Dispersion	1,2 Water-Water
d) Settling	1,2 Water-Water or Water-Bed
e) Erosion	3 Surface Bed-Water
f) Pore Water Diffusion	3,4 Surface Bed-Water or Bed-Bed
g) Sediment Turnover	3 Surface Bed-Water
h) Percolation	4 Bed-Bed or Bed-Water
i) Sedimentation	4 Bed-Bed
j) Volatilization	1 Surface Water

Figure 38. TOXIWASP chemical transport and redistribution processes.

segments. Dispersive flows in the bed are diminished by porosity and tortuosity, as given by equation 102. Diffusion coefficients, cross-sectional areas, and characteristic lengths can be specified as standard WASP input. Tortuosity must be included in the value specified for characteristic length:

$$\ell'_{ij} = \ell_{ij} \cdot t_{ij} \qquad 110$$

where:

ℓ'_{ij} = characteristic mixing length input for benthic segments i and j, L

ℓ_{ij} = length between midpoints of benthic segments i and j, L

t_{ij} = average tortuosity of benthic segments i and j, L_{water}/L

The average porosity of benthic segments i and j is automatically considered by WASP in calculating pore water diffusion. Porosities are calculated internally from sediment concentrations and set to dry weight ratios:

$$n_j = (P-1) \cdot S \qquad 111$$

where:

P = sediment wet weight to dry weight ratio, M (sediment + water)/M (sediment)

1.5.3.2 Chemical Loading

Chemical loading can occur from a variety of sources, including municipal and industrial wastewater discharges; spills and leaks during chemical manufacture, transport, and use; urban runoff and combined sewer overflow; agricultural and mining runoff; precipitation and atmospheric deposition; and subsurface runoff. The largest source of uncertainty in many chemical simulations is in the loading estimate. Both the magnitude and variability may be poorly characterized, and even the existence or location of a chemical discharge may be in doubt. These chemical loadings must be measured or estimated and input into each segment as a steady or time-variable load using standard WASP input. Daily pesticide runoff loads can be simulated with a watershed model and read in directly from an appropriately formatted nonpoint source loading file.

1.5.3.3 Benthic Exchange

Chemical exchange across the benthic interface can be caused by scour, deposition, pore water advection, pore water diffusion, and equilibration (sorption or desorption) with surficial sediments mixed upward through bioturbation. These processes are included in the following functional form, where positive loading is defined from surficial benthic segment i to water segment j.

$$\begin{aligned} W_{Bcij} &= A_{ij} \cdot (w_R \cdot S_i\, C'_{si} - w_D \cdot S_j \cdot C'_{sj}) \\ &+ Q_{ij} \cdot C'_{wij} + R_{Bij} \cdot (C'_{wi} - C'_{wj}) \\ &+ T_{ij} \cdot (C'_{si} - K_{pi} \cdot C'_{wj}) \qquad 112 \end{aligned}$$

where:

T_{ij} = sediment turnover rate, M/T

The scour and deposition of sorbed chemical C'_s is driven by sediment scour and deposition (equation 104), discussed in an earlier section. In TOXIWASP, steady pore water flows input for a subsurface benthic segment using parameter WS(ISEG) are automatically routed through the overlying benthic segments to the water column. Positive (upward) flows carry dissolved benthic concentration C'_{wi}, whereas negative (downward) flows carry dissolved water concentration C_{wj}. Diffusive pore water exchange with the water column R_{Bij}, as modified by porosity and tortuosity, is given by equation 102. Diffusion coefficients, cross-sectional areas, and characteristic lengths corrected for tortuosity are specified as standard WASP input.

Finally, benthic exchange may result from direct sorption and desorption of chemical between surficial sediment and overlying water. These rates are usually rapid. When the active benthic layer is deeper due to physical mixing or bioturbation, then sorptive exchange may be limited by the supply of "new" solids to the surface. Physical and biological mixing of sediment and sorbed chemical from within the bed to the surface is represented in TOXIWASP by a sediment turnover rate proportional to surficial pore water dispersion:

$$T_{ij} = f_T \cdot R_{Bij} \cdot S'_i \qquad 113$$

where:

f_T = the spatially variable proportionality constant between pore water dispersion and sediment mixing (0-1)

S'_i = sediment concentration per unit pore water, M/L^3_w

Proportionality constants f_T can be input to surficial bed segments using parameter DSPSED(ISEG). For quiescent waters with little bioturbation, f_T approaches 0 and direct sorption onto surficial sediments is unimportant. For benthic environments with high bioturbation rates controlling both pore water dispersion and sediment mixing, f_T approaches 1. For turbulent waters with high scour and deposition, pore water dispersion and direct sorption should diminish in importance.

1.5.3.4 Bed Sedimentation and Erosion

Sorbed chemical in the bed migrates downward or upward with respect to the bed surface in response to net sedimentation or erosion. This is represented by the term W_{sed} in governing equation 101. W_{sed} is calculated internally following equation 107, and implemented by the scheme described in Section 1.5.2.4.

Dissolved chemical in the bed also migrates with the sedimentation velocity. If the density of the bed increases with depth, compaction squeezes pore water flow upward carrying dissolved chemical. This is represented by the term Q_{ps} in governing equation 101. Q_{ps} is calculated internally following equation 106, and implemented by the scheme described in Section 1.5.2.4.

1.5.3.5 Equilibrium Sorption

Dissolved chemical in water column and benthic segments interacts with sediment particulates and biomass to form three phases--dissolved, sorbed, and biosorbed. The reactions can be written with respect to unit volume of water:

$$S' + C_w' = C_s/n \qquad 114$$

$$B' + C_w' = C_B/n \qquad 115$$

The forward reaction is sorption and the backward reaction is desorption. These reactions are usually fast in comparison with the model time step, and can be considered in local equilibrium. The phase concentrations C_w, C_s, and C_B are governed by the equilibrium partition coefficients K_{ps} and K_{pB} (L/kg):

$$K_{ps} = \frac{C_s/n}{S' \cdot C_w'} = \frac{C_s'}{C_w'} \qquad 116$$

$$K_{pB} = \frac{C_B/n}{B' \cdot C_w'} = \frac{C_B'}{C_w'} \qquad 117$$

These equations give the linear form of the Freundlich isotherm, applicable when sorption sites on sediment and biota are plentiful:

$$C_s' = K_{ps} \cdot C_w' \qquad 118$$

$$C_B' = K_{pB} \cdot C_w' \qquad 119$$

The partition coefficients depend upon characteristics of the chemical and the sediments or biomass onto which sorption has occurred. Many organic pollutants of current interest are non-polar, hydrophobic compounds whose partition coefficients correlate quite well with the organic fraction of the sediment. Rao and Davidson (1980) and Karickhoff et al. (1979) have developed empirical expressions relating equilibrium coefficients to laboratory measurements leading to fairly reliable means of estimating appropriate values. The correlations used in TOXIWASP are

$$K_{ps} = K_{oc} \cdot f_{ocs} \qquad 120$$

$$K_{pB} = K_{oc} \cdot f_{ocB} \qquad 121$$

where:

K_{oc} = organic carbon partition coefficient, (L_w/kg_{oc})

f_{ocs} = organic carbon fraction of sediment

f_{ocB} = organic carbon fraction of biomass

The spatially variable values of f_{ocs} are input using parameter OCS(ISEG). The value of f_{ocB} is input using constant OCB. The value of K_{oc} is input using constant KOC. If no K_{oc} values are available, one is generated internally using the following correlation with the octanal-water partition coefficient K_{ow} (L_w/L_{oct}):

$$K_{oc} = 0.41 \cdot K_{ow} \qquad 122$$

The value of K_{ow} is input using constant KOW.

The total chemical concentration is the sum of the three phase concentrations

$$C = C_w' \cdot n + C_s' \cdot S + C_B' \cdot B \qquad 123$$

Substituting equations 118 and 119, factoring, and rearranging terms gives the dissolved fraction α_1:

$$\alpha_1 = \frac{C_w' \cdot n}{C} = \frac{1}{1 + K_{ps} \cdot S/n + K_p \cdot B/n} \qquad 124$$

Similarly, the sorbed and biosorbed fractions are

$$\alpha_2 = \frac{C_s' \cdot S}{C} = \frac{K_{ps} \cdot S/n}{1 + K_{ps} \cdot S/n + K_{pB} \cdot B/n} \qquad 125$$

$$\alpha_3 = \frac{C_B' \cdot B}{C} = \frac{K_{pB} \cdot B/n}{1 + K_{ps} \cdot S/n + K_{pB} \cdot B/n} \qquad 126$$

These fractions are determined in time and space throughout a simulation from the partition coefficients, internally, calculated porosities (equation 111), simulated sediment concentrations, and specified biomass concentrations. The latter are input using parameter BIOMAS(ISEG).

Given the total concentration and the three phase fractions, the dissolved, sorbed, and biosorbed concentrations are uniquely determined:

$$C_w = C \cdot \alpha_1 \qquad 127$$

$$C_s = C \cdot \alpha_2 \qquad 128$$

$$C_B = C \cdot \alpha_3 \qquad 129$$

These three concentrations have units of mg/L, and are named CHEM1, CHEM2, and CHEM3. These can be expressed as concentrations within each phase:

$$C_w' = C_w/n \qquad 130$$

$$C_s' = C_s/S \qquad 131$$

$$C'_B = C_B/B \qquad 132$$

These concentrations have units of mg/L_w, mg/kgs, and mg/kg_B, respectively, and are named CHEMW, CHEMS, and CHEMB.

In some cases, such as near discharges, the user may have to alter input partition coefficients to describe the effect of incomplete sorption. As guidance, Karickhoff and Morris (1985) found that typical sorption reaction times are related to the partition coefficient:

$$k_d^{-1} = 0.03 \cdot K_{ps} \qquad 134$$

where:

k_d = desorption rate constant, hr^{-1}

Thus, compounds with high, medium, and low K_{ow}'s of 10^5, 10^3, and 10 sorbing onto 2% organic sediment should have reaction times of a day, a half hour, and seconds.

TOXIWASP data specifications for sorption are summarized in Figure 39.

1.5.3.6 Kinetic Transformation

Dissolved, sorbed, and biosorbed chemical in water column and benthic segments are subject to several transformation processes. Several variables may be influencing each process, leading to a multi-term and often non-linear lumped transformation rate. To make this problem tractible, TOXIWASP uses the strategy implemented in the original Exposure Analysis Modeling System (Burns et al., 1982). Each process is considered separately using mixed second order kinetics:

$$C + [E]_k \text{ ----> } P_i \qquad 134$$

where:

$[E]_k$ = the intensity of environmental property affecting process "k," such as light intensity or bacterial population

P_i = transformation product for process k

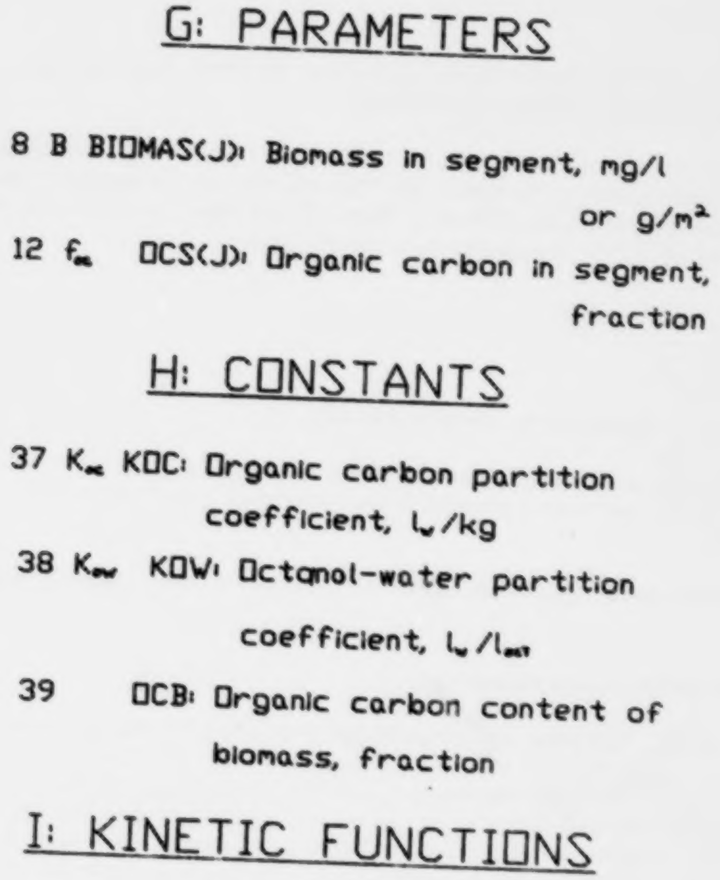
The reaction rate S_{kc} in mg/L-day for process k is:

$$S_{kc} = k_k \cdot [E]_k \cdot Y_k \cdot C \qquad 135$$

where:

k_k = second-order rate constant for process k

Y_k = yield coefficient for process k



G: PARAMETERS

8 B BIOMAS(J): Biomass in segment, mg/l or g/m^2

12 f_{oc} OCS(J): Organic carbon in segment, fraction

H: CONSTANTS

37 K_{oc} KOC: Organic carbon partition coefficient, l_w/kg

38 K_{ow} KOW: Octanol-water partition coefficient, l_w/l_{oct}

39 OCB: Organic carbon content of biomass, fraction

I: KINETIC FUNCTIONS

Figure 39. TOXIWASP sorption data.

Given a local value for $[E]_k$, a pseudo-first order rate coefficient K_k in day^{-1} can be specified:

$$K_k = k_k \cdot [E]_k \cdot Y_k \qquad 136$$

For a compound undergoing several competing reactions, the lumped first order reaction coefficient K in day^{-1} is

$$K = \sum_k K_k \qquad 137$$

and

$$S_{kc} = K \cdot C \qquad 138$$

This local first order assumption is generally accepted to be accurate for most chemicals at environmental concentrations. The assumption is invalid at concentrations near the solubility limit, however. If the user does not specify a maximum concentration CMAX(1) (in Data Group K), TOXIWASP sets this limit at half the solubility or 10^{-5} molar, whichever is less, and aborts the simulation if concentrations exceed this value.

The individual transformation processes considered by TOXIWASP are hydrolysis, photolysis, oxidation, and microbial degradation. In addition, volatilization is calculated and added to the transformation rate. Good discussions of these processes have been published, for example Smith et al. (1977), Burns et al. (1982), Mill et al. (1982), Mabey et al. (1982), and Mills et al. (1985). The following sections summarize how TOXIWASP calculates the local rate constant for each of these processes. Input data requirements are given for each process. The general kinetic data required by TOXIWASP are summarized in Figure 40.

Hydrolysis--

Hydrolysis, or reaction of the chemical with water, is known to be a major pathway for degradation of many toxic organics. An example reaction is shown in Figure 41. The reaction can be catalyzed by hydrogen and hydroxide ions. Figure 42 illustrates the effects of acid, base, and neutral hydrolysis on parathion, base hydrolysis on carbaryl, neutral hydrolysis on chloromethane, and acid and base hydrolysis on 2,4-D.

In TOXIWASP, hydrolysis by specific-acid-catalyzed, neutral, or specific-base-catalyzed pathways is considered for dissolved, sorbed, and biosorbed chemical:

$$\begin{aligned} K_H = {} & (k_a^1\,[H^+] + k_n^1 + k_b^1\,[OH^-]) \cdot \alpha_1 \\ & + (k_a^2\,[H^+] + k_n^1 + k_b^2\,[OH^-]) \cdot \alpha_2 \\ & + (k_a^3\,[H^+] + k_n^3 + k_b^3\,[OH^-]) \cdot \alpha_3 \end{aligned} \qquad 139$$

where:

K_H = net hydrolysis rate constant, hr^{-1}

k_a, k_b = specific acid and base catalyzed rate constants, respectively, $molar^{-1} \cdot hr^{-1}$

k_n = neutral rate constant, hr^{-1}

subscripts 1,2,3 = dissolved, sorbed, biosorbed phases

α_1, α_2, α_3 = fraction of chemical in each phase

TOXIWASP hydrolysis data specifications are summarized in Figure 43. The nine reaction coefficients can be specified as constants 10-18, with

G: PARAMETERS

1 T TEMPM(J) Segment temperature, °c

2 d DEPTHG(J) Segment depth, ft

18 K_T TOTKG(J) Total first-order decay rate (optional), day^{-1}

H:CONSTANTS

47 SOLG Solubility of chemical in water, mg/l

48 ESOLG Solubility temperature correction, kcal/g-mole

43 MWTG Molecular weight of compound

I: KINETIC FUNCTIONS

1 TEMPN Normalized temperature

Figure 40. TOXIWASP general kinetic data.

activation energy constants 1-9 left as 0. If the user wants TOXIWASP to determine rates based on the temperature-based Arrhenius function, then non-zero activation energies specified as constants 1-9 will invoke the following calculation for each rate constant k.

$$k = 10^{(\log A) - 1000.E_a/4.58.T_k} \tag{140}$$

where:

A = pre-exponential, or "frequency factor"

E_a = Arrhenius activation energy, kcal/mole

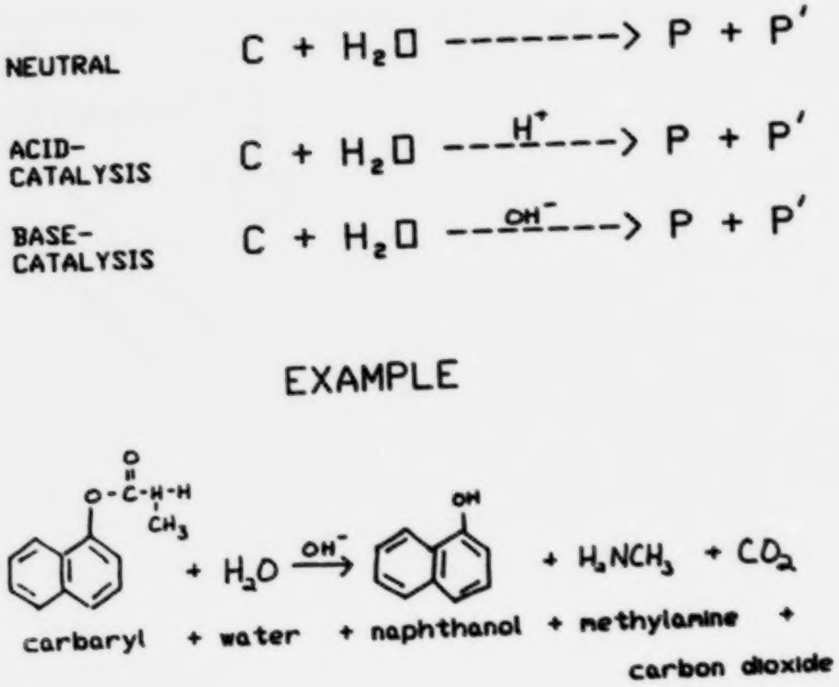

NEUTRAL
C + H₂O -------> P + P′
ACID-CATALYSIS
C + H₂O ---H⁺---> P + P′
BASE-CATALYSIS
C + H₂O ---OH⁻---> P + P′
EXAMPLE
O
O-C-N-H
CH₃
+ H₂O
OH⁻
OH
+ H₂NCH₃
+ CO₂
carbaryl
+ water
+ naphthanol
+ methylamine
+ carbon dioxide

Figure 41. Hydrolysis.

4.58 = 2.303 . R, cal/mole-°K

T_k = water temperature, °K

The log of the frequency factor is specified using constants 10-15. They can be calculated from known activation energies and reaction rates observed at a particular temperature:

$$\log A = \log k + \frac{1000 \cdot E_a}{4.58 \cdot T_k} \qquad 141$$

Thus, if a dissolved neutral hydrolysis rate of $2.38 \cdot 10^{-4}$ hr^{-1} was observed at 25°C, an activation energy of 20 kcal/mole would give a log frequency factor of 11.03. If this value is entered as constant 16, 20 kcal/mole is entered as constant 4, and water temperatures of 25 and 20°C are specified for two segments, then TOXIWASP will use equation 139 to calculate rate constants of $2.38 \cdot 10^{-4}$ hr^{-1} and $1.34 \cdot 10^{-4}$ hr^{-1}, respectively.

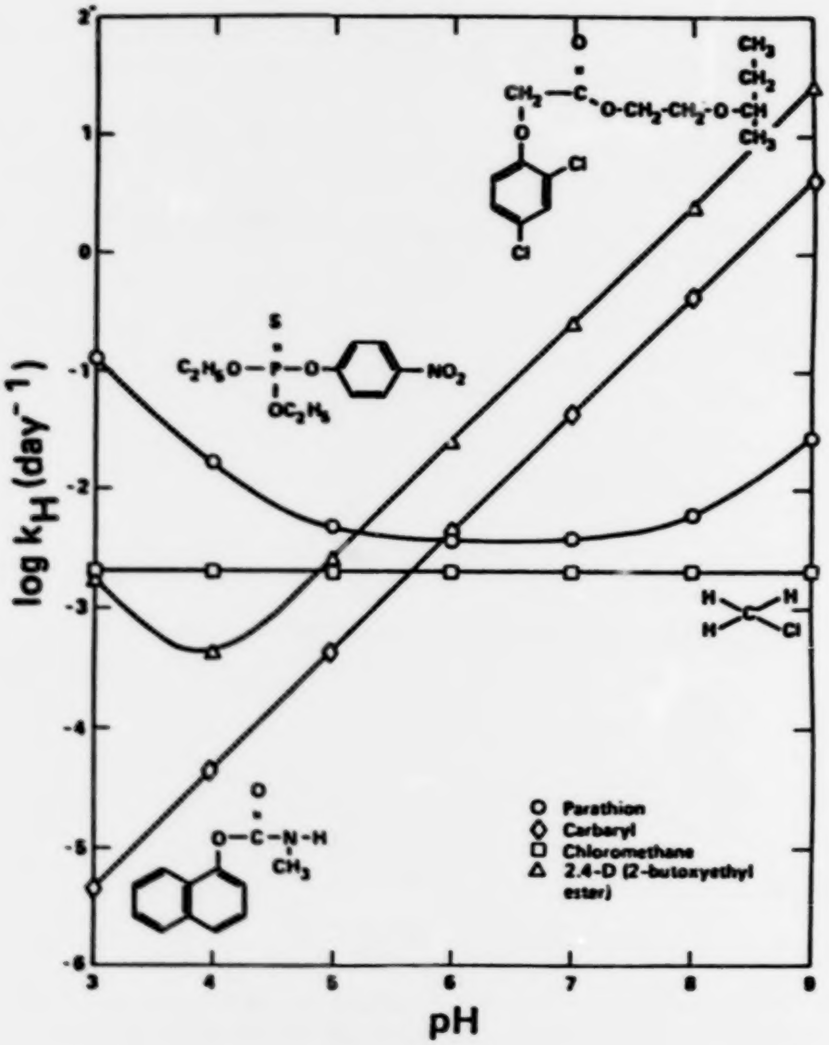


Figure 42. pH dependence of hydrolysis rate constants.

Photolysis

Photolysis is the transformation of a chemical due to absorption of light energy. An example of several photochemical pathways is given in Figure 44. The first order rate coefficient for photolysis can be calculated from the absorption rate and the quantum yield for each phase:

G: PARAMETERS

10	pOH	POHG(J): hydroxide ion activity (avg)
15	pH	PHG(J): hydrogen ion activity (avg)

H: CONSTANTS

1,2,3	EBHG(I,1): Arrhenius activation energy, base, kcal/mol
4,5,6	ENHG(I,1): Arrhenius activation energy, neutral
7,8,9	EAHG(I,1): Arrhenius activation energy, acid
13,14,15	KBHG(I,1): Base hydrolysis rate constant, mol^{-1} hr
16,17,18	KNHG(I,1): Neutral hydrolysis rate constant, hr^{-1}
10,11,12	KAHG(I,1): Acid hydrolysis rate constant, mol^{-1} hr

I: KINETIC FUNCTIONS

3	PHN: Normalized pH
4	POHN: Normalized pOH

Figure 43. TOXIWASP hydrolysis data.

$$K_{pG} = \sum_{i=1}^{3} k_{ai} \cdot \phi_i \cdot \alpha_i \qquad 142$$

where:

K_{pG} = first order photolysis rate coefficient at reference light intensity, hr^{-1}

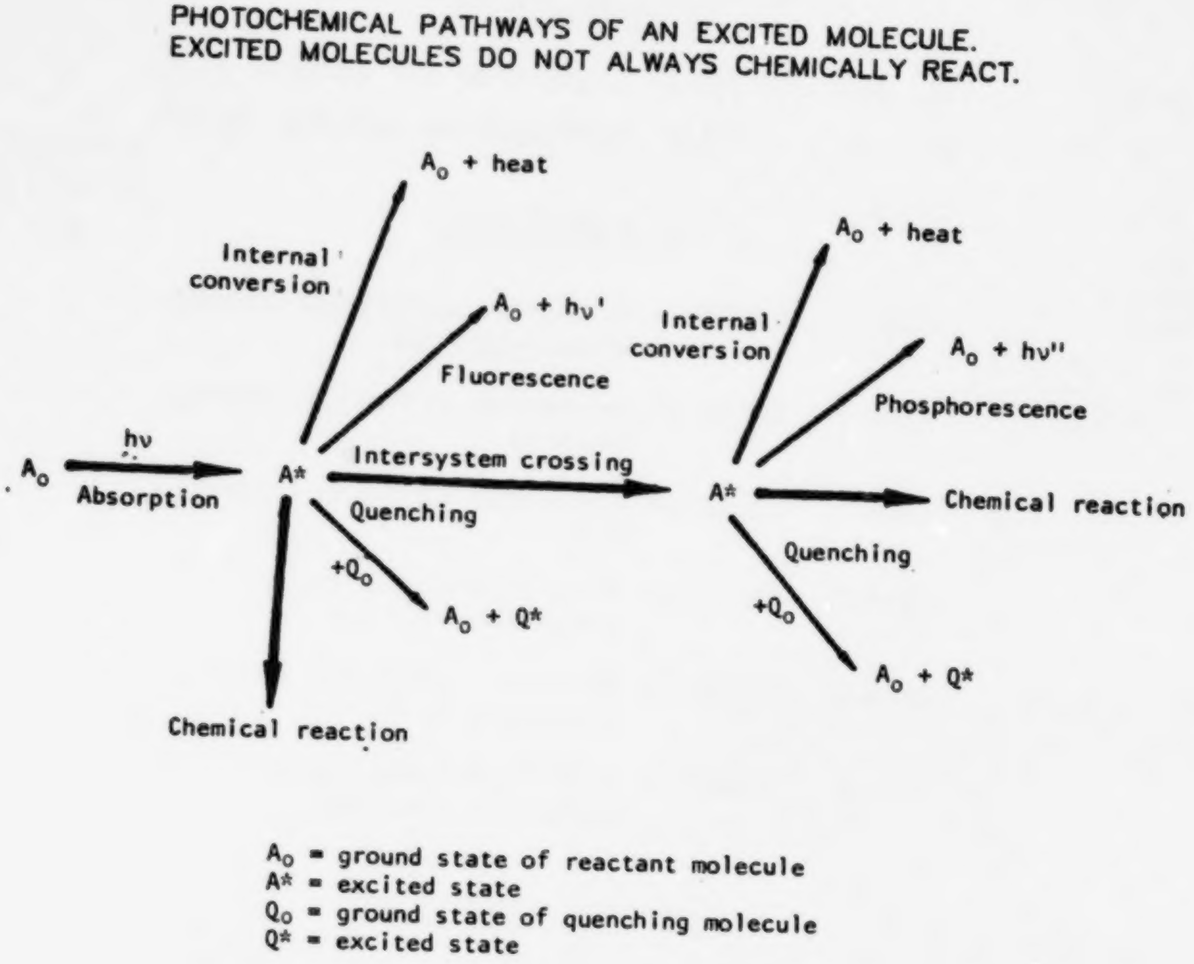

PHOTOCHEMICAL PATHWAYS OF AN EXCITED MOLECULE.
EXCITED MOLECULES DO NOT ALWAYS CHEMICALLY REACT.
A_o + heat
Internal conversion
A_o + hν'
Fluorescence
hν
A_o
Absorption
A*
Intersystem crossing
Quenching
$+Q_o$
A_o + Q*
Chemical reaction
A_o + heat
Internal conversion
A_o + hν''
Phosphorescence
A*
Chemical reaction
Quenching
$+Q_o$
A_o + Q*
A_o = ground state of reactant molecule
A* = excited state
Q_o = ground state of quenching molecule
Q* = excited state

Figure 44. Photolysis.

k_{ai} = specific sunlight absorption rate for phase i, E/mole-hr or (E/L)/(mole/L)/hr

α_i = fraction of chemical in phase i

The specific sunlight absorption rate is the integral or summation over all bandwidths of the average light multiplied by the molar absorptivity and the optical path:

$$k_a = \sum I_{Gk} \cdot \varepsilon_k \cdot d \cdot 2300 \cdot 3600$$

where:

I_{Gk} = average light intensity of wavelength k, E/cm^2-sec

ϵ_k = molar absorptivity of wavelength k, m 10-L/cm . mole

d = optical path, cm/cm

$$2300 = \frac{cm^3}{L.\ln 10}$$

$$3600 = \frac{sec}{hr}$$

TOXIWASP does not make the above calculations for the first order rate coefficient under reference light conditions. The user must supply this rate coefficient, calculated or measured for near surface waters during cloudless conditions. TOXIWASP extrapolates this coefficient to ambient light conditions with the following calculation.

$$K_p = K_{pG} \cdot [L] \cdot \sum_{i=1}^{3} \phi_{pi} \cdot \alpha_i \qquad 144$$

where:

[L] = fraction of reference light I_G in segment (I_m/I_G)

ϕ_{pi} = reaction yield fraction for chemical in phase i

The reference light fraction in a segment accounts for spatially-variable light extinction, cloud cover, latitude changes, and surface light variability:

$$[L] = \frac{I_m}{I_o} \cdot (1-0.056.C_G) \cdot L_c \cdot \left(\frac{I_o(t)}{I_G}\right) \qquad 145$$

where:

I_m = average light intensity within water segment, E/cm^2-sec

I_o = surface light intensity, E/cm^2-sec

C_G = cloud cover, tenths of sky (1-10)

0.056 = average cloud reduction factor

L_c = latitude correction factor, calculated internally

Light extinction is calculated with the integrated Beer-Lambert formulation:

$$\frac{I_m}{I_o} = \frac{1 - e^{-d.K_e.D}}{d \,.\, K_e \,.\, D} \qquad 146$$

where:

K_e = spatially variable light extinction coefficient, m^{-1}

D = depth of water segent, m

The time variable surface light relative to the reference light is input as time function LIGHTN. This can be used to represent diurnal or seasonal changes. TOXIWASP photolysis data specifications are summarized in Figure 45.

Oxidation

Chemical oxidation of organic toxicants in aquatic systems can be a consequence of interactions between free radicals and the pollutants. Free radicals can be formed as a result of photochemical reactions. Free radicals that have received some attention in the literature include alkylperoxy radicals, RO_2.; OH radicals; and singlet oxygen.

In TOXIWASP, oxidation is modeled as a general second-order process for dissolved, sorbed, and biosorbed chemical:

$$[RO_2] \,.\, \sum_{i=1}^{3} k_o^i \,.\, \alpha_i \qquad 147$$

where:

K_o = net oxidation rate constant, hr^{-1}

$[RO_2]$ = molar concentration of oxidant, moles/L

k_o^i = second order oxidation rate constant for chemical phase i, L/mole-hr

Because of the large number of alkylperoxy radicals that potentially exist in the environment, it would be impossible to obtain estimates of k_{ox} for each species. Mill et al. (1982) propose estimation of a rate coefficient using t-butyl hydroperoxide as a model oxidizing agent. They argue that other alkylperoxides exhibit similar reactivities to within an order of magnitude. The three second-order rate coefficients are input to TOXIWASP using KOXG(I), constants 22-24.

In addition to estimating a rate coefficient, an estimate of free radical concentrations must be made to completely define the expression for free

G: PARAMETERS

17 K_e CMPETG(J): Light extinction coefficient, m^{-1}

H: CONSTANTS

54 KDPG: Near-surface photolytic rate constant, hr^{-1}

55 RFLAT: Reference latitude for KDPG, deg

56 CLOUDG: Average cloudiness, tenths of sky

57 LATG: Latitude of water body, deg

58 DFACG: Ratio of optical path/depth

59,60,61 QUANTG(I): Reaction quantum yield for dissolved, sorbed, biosorbed

I: KINETIC FUNCTIONS

5 LIGHTN: Normalized light intensity

Figure 45. TOXIWASP photolysis data.

radical oxidation. Mill et al. (1982) report RO_2 concentrations on the order of 10^{-9} $\underline{M}$ and OH concentrations on the order of 10^{-17} $\underline{M}$ for a limited number of water bodies. Zepp et al. (1977) report an average value on the order of 10^{-12} $\underline{M}$ for singlet oxygen in water bodies sampled. The source of free radicals in natural waters is photolysis of naturally occurring organic molecules. If a water body is turbid or very deep, free radicals are likely to be generated only near the air-water interface, and consequently, chemical oxidation will be relatively less important.

In such cases, the concentrations cited above are appropriate in only the near-surface zones of water bodies. The molar oxidant concentrations are input to TOXIWASP using parameter OXRADG(ISEG).

Bacterial Degradation

Bacterial degradation, sometimes referred to as microbial transformation, biodegradation or biolysis, is the breakdown of a compound by the enzyme systems in bacteria. Examples are given in Figure 46. Although these transformations can detoxify and mineralize toxins and defuse potential toxins, they can also activate potential toxins.

Two general types of biodegradation are recognized--growth metabolism and cometabolism. Growth metobolism occurs when the organic compound serves as a food source for the bacteria. Adaptation times from 2 to 50 days are generally required. Bacterial adaptation is faster for chronic exposure and higher microbial poulations. Adaptation is slower for low populations or when easily degradable carbon sources are present. Following adaptation, biodegradation proceeds at fast first-order rates. Cometabolism occurs when the organic compound is not a food source for the bacteria. Adaptation is seldom necessary, and the transformation rates are slow compared with growth metabolism.

In TOXIWASP, biodegradation is limited to cometabolism. It is assumed that bacterial populations are unaffected by the presence of the compound at low concentrations. Second-order kinetics for dissolved, sorbed, and biosorbed chemical in the water column and the bed are considered:

$$K_{Bw} = P_{bac} \cdot f_B \cdot \sum_{i=1}^{3} k_{Bw}^{i} \cdot \alpha_i \qquad 148$$

$$K_{Bs} = P_{bac} \cdot f_B \cdot \sum_{i=1}^{3} k_{Bs}^{i} \cdot \alpha_i \qquad 149$$

where:

K_{Bw} = net biodegradation rate constant in water segment, hr^{-1}

K_{Bs} = net biodegradation rate constant in benthic segment, hr^{-1}

k_{Bw}^{i} = second order biodegradation rate constant for phase i in water segments, ml/cell-hr

k_{Bs}^{i} = second order biodegradation rate constant for phase i in benthic segments, ml/cell-hr

P_{bac} = bacterial population density in segment, cell/ml

f_B = fraction of population actively degrading organic compound

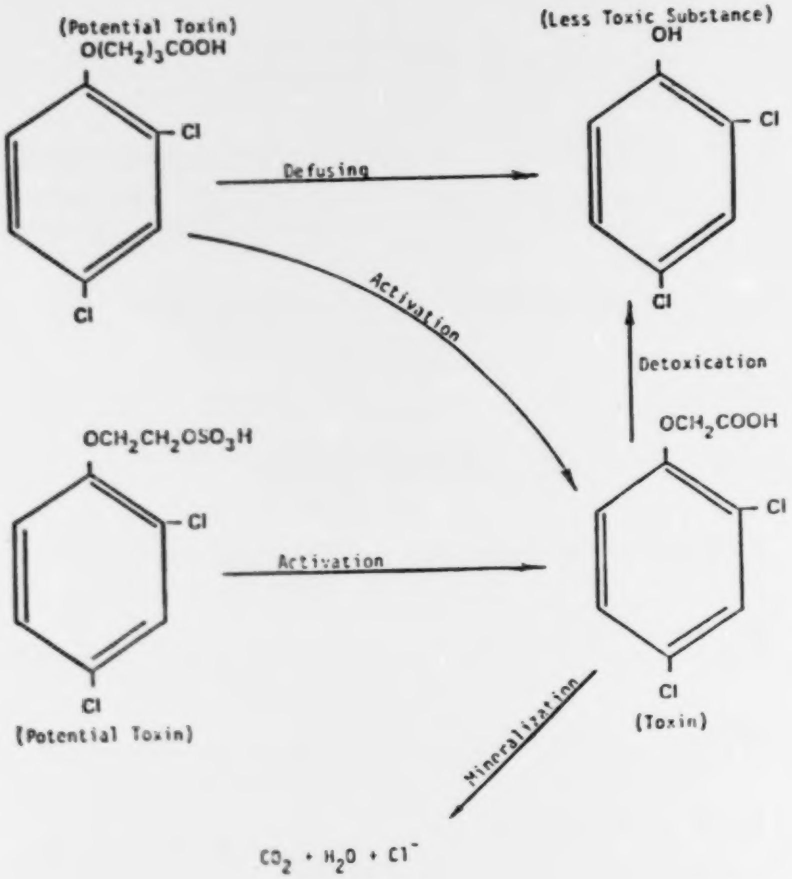

(Potential Toxin)
$O(CH_2)_3COOH$
Cl
Cl
Defusing
(Less Toxic Substance)
OH
Cl
Cl
Activation
Detoxication
$OCH_2CH_2OSO_3H$
Cl
Cl
(Potential Toxin)
Activation
OCH_2COOH
Cl
Cl
(Toxin)
Mineralization
$CO_2 + H_2O + Cl^-$

Figure 46. Microbial transformations of toxic chemicals (Alexander 1980).

TOXIWASP biodegradation data specifications are summarized in Figure 47. The three second order rate constants for water and for bed segments can be specified as constants 25-27 and 31-33. Temperature correction factors can be left at 0. If the user wants TOXIWASP to correct the rate constants for ambient segment temperatures, then nonzero temperature correction factors specified as constants 28-30 and 34-36 will invoke the following modification for each rate constant k_B.

$$k_{Bw}(T) = k_{Bw} \cdot Q_{Tw}^{(T-20)/10} \tag{150}$$

$$k_{Bs}(T) = k_{Bs} \cdot Q_{Ts}^{(T-20)/10} \tag{151}$$

G: PARAMETERS

6	BACTOG(J)	Bacterial population cells/ml (water) cells/100g (bed)
7	ACBAC(J)	Active fraction of bacteria

H: CONSTANTS

25,26,27	KBACWG(I,1)	Water-column rate constant, ml/cell
28,29,30	QTBAWG(I,1)	Temperature correction factor
31,32,33	KBACSG(I,1)	Benthic rate constant, ml/cell-hr
34,35,36	QTBASG	Temperature correction factor

Figure 47. TOXIWASP bacterial degradation parameters.

where:

Q_{Tw} = "Q-10" temperature correction factor for biodegradation in water

Q_{Ts} = "Q-10" temperature correction factor for biodegradation in benthic segments

T = ambient temperature in segment, °C

The temperature correction factors represent the increase in the biodegradation rate constants resulting from a 10°C temperature increase. Values in the range of 1.5 to 2 are common.

Total bacterial populations for water and benthic segments are input using parameter BACTOG(ISEG). Typical population size ranges are given in Table 14. Note that input units for benthic segments are cells/100 g dry weight. These are corrected to cells/ml internally. The total population counts are reduced by the spatially variable active bacterial fraction, input through parameter ACBAC(ISEG).

TABLE 14. SIZE OF TYPICAL BACTERIAL POPULATIONS IN NATURAL WATERS

Water Body Type	Bacterial Numbers (cells/ml)	Ref.
Oligotrophic Lake	50 - 300	a
Mesotrophic Lake	450 - 1,400	a
Eutrophic Lake	2000 - 12,000	a
Eutrophic Reservoir	1000 - 58,000	a
Dystrophic Lake	400 - 2,300	a
Lake Surficial Sediments	8×10^9 - 5×10^{10} cells/g dry wt	a
40 Surface Waters	500 - 1×10^6	b
Stream Sediments	10^7 - 10^8 cells/g	c
Rur River (winter)	3×10^4	d

References:

[a] Wetzel (1975). Enumeration techniques unclear.

[b] Paris *et al*. (1981). Bacterial enumeration using plate counts.

[c] Herbes & Schwall (1978). Bacterial enumeration using plate counts.

[d] Larson *et al*. (1981). Bacterial enumeration using plate counts.

Environmental factors other than temperature and population size can limit bacterial rates. Potential reduction factors must be considered externally by the user, and input through parameter ACBAC(ISEG). Nutrient limitation can be important in oligotrophic environments. The following reduction factor was used by Ward and Brock (1976) to describe phosphate limitation of hydrocarbon degradation:

$$f_{PO4} = \frac{0.0277 \cdot C_{PO4}}{1 + 0.0277 \cdot C_{PO4}} \qquad 152$$

where:

C_{PO4} = dissolved inorganic phosphorus concentration, ug/L

Low concentrations of dissolved oxygen can cause reductions in biodegradation rates. Below DO concentrations of about 1 mg/L, the rates start to decrease. When anoxic conditions prevail, most organic substances are biodegraded more slowly. Because biodegradation reactions are generally more difficult to predict than physical and chemical reactions, site-specific calibration becomes more important. TOXIWASP allows several methods to correct rates to reflect field data.

Volatilization

Volatilization is the movement of chemical across the air-water interface. The dissolved neutral concentration attempts to equilibrate with the gas phase partial pressure, as illustrated in Figure 48. The equation in this figure shows that equilibrium occurs when the dissolved concentration equals the partial pressure divided by Henry's Law Constant. In most cases, organic toxicants in the atmosphere are at much lower levels than partial pressures equilibrated with water concentrations. Consequently, volatilization reduces to a first-order process with a rate proportional to the conductivity and surface area divided by volume:

$$K_v = k_v \cdot \frac{A_s}{V} \cdot \alpha_1 = k_v \cdot \frac{\alpha_1}{D} \qquad 153$$

where:

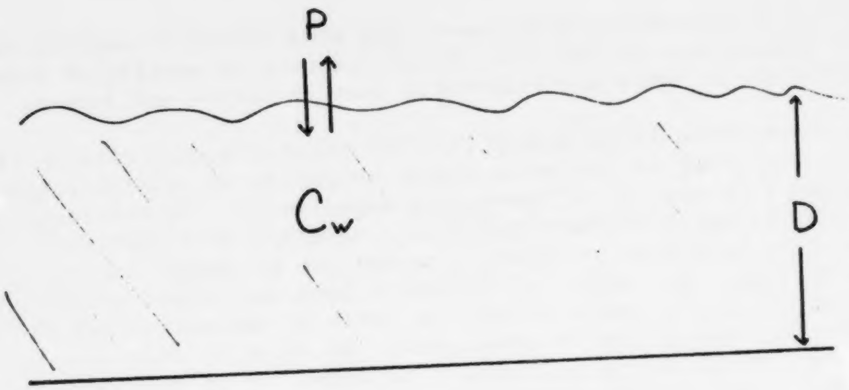
K_v = net volatilization rate constant, hr^{-1}

k_v = conductivity of the chemical through the water segment, m/hr

A_s = surface area of water segment, m^2

V = volume of the water segment, m^3

D = average depth of the segment, m



$$\frac{\partial C_w}{\partial t} = -\frac{k_v}{D}\left(C_w - \frac{P}{H}\right)$$

C_w = DISSOLVED CONCENTRATION, mg/l

P = PARTIAL PRESSURE, atm

H = HENRY'S LAW CONSTANT, $\frac{atm}{M}$

D = DEPTH, m

k_v = RATE CONSTANT, m/hr (conductivity)

Figure 48. Volatilization.

α_1 = dissolved fraction of the chemical

The value of k_v, the conductivity, depends on the intensity of turbulence in a water body and in the overlying atmosphere. Mackay and Leinonen (1975) have discussed conditions under which the value of k_v is primarily determined by the intensity of turbulence in the water. As the Henry's Law coefficient increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. As the Henry's Law coefficient decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

Because Henry's Law coefficient generally increases with increasing vapor pressure of a compound and generally decreases with increasing solubility of a compound, highly volatile low solubility compounds are most likely to exhibit mass transfer limitations in water and relatively nonvolatile high solubility compounds are more likely to exhibit mass transfer limitations in the air. Volatilization is usually of relatively less magnitude in lakes and reservoirs than in rivers and streams.

In cases where it is likely that the volatilization rate is regulated by turbulence level in the water phase, estimates of volatilization can be obtained from results of laboratory experiments. As discussed by Mill et al. (1982), small flasks containing a solution of a pesticide dissolved in water that have been stripped of oxygen can be shaken for specified periods of time. The amount of pollutant lost and oxygen gained through volatilization can be measured and the ratio of conductivities (KVOB) for pollutants and oxygen can be calculated. As shown by Tsivoglou and Wallace (1972), this ratio should be constant irrespective of the turbulence in a water body. Thus, if the reaeration coefficient for a receiving water body is known or can be estimated and the ratio of the conductivity for the pollutant to reaeration coefficient has been measured, the pollutant conductivity can be estimated.

In TOXIWASP, the dissolved concentration of a compound in a surface water column segment can volatilize at a rate determined by the two-layer resistance model (Whitman, 1923), where the conductivity is the reciprocal of the total resistance:

$$k_v = (R_L + R_G)^{-1} \qquad 154$$

where:

R_L = liquid phase resistance, hr/m

R_G = gas phase resistance, hr/m

The two-resistance method assumes that two "stagnant films" are bounded on either side by well mixed compartments. Concentration differences serve as the driving force for the water layer diffusion. Pressure differences drive the diffusion for the air layer. From mass balance considerations, it is obvious that the same mass must pass through both films, thus the two resistances combine in series. There is actually yet another resistance involved, the transport resistance between the two interfaces, but it is assumed to be negligible. This may not be true in two cases: very turbulent conditions and in the presence of surfaceactive contaminants. Although this two-resistance method, the Whitman model, is rather simplied in its assumption of uniform layers, it has been shown to be as accurate as more complex models. Laboratory studies of volatilization of organic chemicals confirm the validity of the method as an accurate predictive tool (Burns et al., 1982).

In TOXIWASP, the liquid phase resistance to the compound is assumed to be proportional to the transfer rate of oxygen, which is limited by the liquid phase only:

$$R_L = \frac{1}{K_{o2} \sqrt{32/MW}} \qquad 155$$

where:

K_{o2} = temperature corrected reaeration velocity, m/hr

MW = molecular weight of the compound, g/mole

32 = molecular weight of oxygen, g/mole

If a measured proportionality factor KVOG is available, it is used in place of $\sqrt{32/MW}$. The gas phase resistance to the compound is assumed to be proportional to the transfer rate of water vapor, which is limited by the gas phase only:

$$R_G = \frac{1}{\frac{H}{RT_k} \cdot WAT \cdot \sqrt{18/MW}} \qquad 156$$

where:

WAT = water vapor exchange velocity, m/hr

18 = molecular weight of water, g/mole

H = Henry's Law constant, atm-m^3/mole

R = ideal gas constant = 8.206×10^{-5} m^3-atm/mol°K

T_k = water temperature, °K

The reaeration and water vapor exchange velocities vary with stream reach and time of year. They can be calculated using one of several empirical formulations.

TOXIWASP calculates flow-induced reaeration based on the Covar method (Covar, 1976). This method calculates reaeration as a function of velocity and depth by one of three formulas, Owens, Churchill, or O'Connor-Dobbins, respectively:

$$K_{20} = 0.276 \cdot V^{0.67} \cdot D^{-0.85} \qquad 157$$

$$K_{20} = 0.148 \cdot V^{0.969} \cdot D^{-0.673} \qquad 158$$

$$\text{or} \quad K_{20} = 0.164 \cdot V^{0.5} \cdot D^{-0.5} \qquad 159$$

where:

V = average segment velocity, ft/sec

D = average segment depth, ft

K_{20} = reaeration velocity at 20°C, m/hr

The Owens formula is automatically selected for segments with depth less than 2 feet. For segments deeper than 2 feet, the O'Connor-Dobbins or Churchill formula is selected based on a consideration of depth and velocity. Deeper, slowly moving rivers require O'Connor-Dobbins; moderately shallow, faster moving streams require Churchill.

Whenever the volatilization rate is calculated during a simulation, wind-induced reaeration is determined by

$$K20 = 0.0046 \cdot W + 0.00136 \cdot W^2 \qquad 160$$

where:

W = time-varying windspeed at 10 cm above surface, m/sec

A minimum value of 0.02 m/hr is imposed on K20. Windspeed affects reaeration, then, above 6 m/sec. The reaeration velocity used to compute volatilization is either the flow-induced reaeration or the wind-induced reaeration, whichever is larger. Segment temperatures are used to adjust K20 by the standard formula

$$K_{02} = K20 * 1.024^{(T-20.)} \qquad 161$$

The water vapor exchange velocity used in R_G is calculated using wind speed and a regression proposed by Liss (1973):

$$WAT = 0.1857 + 11.36 \cdot W \qquad 162$$

where:

W = wind speed at 10 cm above surface, m/sec

Wind speed measured above 10 cm must be adjusted to the 10-cm height by the user assuming a logarithmic velocity profile and a roughness height of 1 mm (Israelsen and Hanson, 1962):

$$W = W_z \cdot \log (0.1/0.001)/\log (z/0.001) \qquad 163$$

where:

W_z = wind speed at height z, m/sec

z = measurement height, m

Although there are many calculations involved in determining volatilization, most are performed internally using a small set of data. TOXIWASP volatilization data specifications are summarized in Figure 49. Not all of the constants are required. If Henry's Law constant is unknown, it will be

G: PARAMETERS

3	V	VELOC(J)	Average water velocity, ft/sec
4	W	WINDG(J)	Average wind speed @ 10 cm, m/sec

H: CONSTANTS

44	H	HENRYG	Henry's Law constant, atm-m^3/mol
45		VAPRG	Vapor pressure of chemical, torr
46		KVOG	Ratio of liquid resistance to reaeration rate (measured)
49		EVPRG	Molar heat of vaporation, kcal/mole
50		EHENG	Temperature correction for H, kcal/mole

I: KINETIC FUNCTIONS

2	WINDN	Normalized wind speed

Figure 49. TOXIWASP volatilization data.

calculated internally from vapor pressure and solubility. If KVOG is not measured, it will be calculated internally from molecular weight.

1.5.4 Heavy Metals

Although TOXIWASP was designed explicitly for organic chemicals, it can be used to simulate metals with judicious specification of certain key parameters. Because of the inherent complexity of metals behavior, site-specific calibration is required. Physical processes affecting the fate of metals in rivers are illustrated in Figure 50.

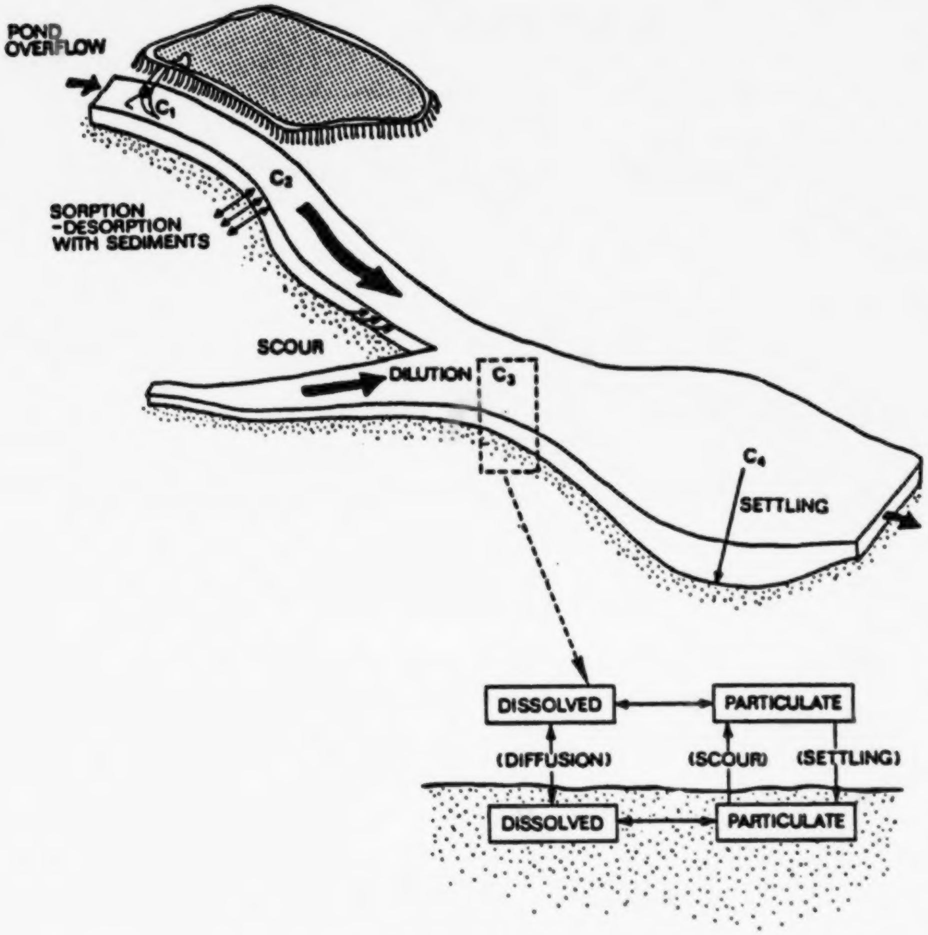

POND OVERFLOW
C_1
C_2
SORPTION -DESORPTION WITH SEDIMENTS
SCOUR
DILUTION
C_3
C_4
SETTLING
DISSOLVED
PARTICULATE
(DIFFUSION)
(SCOUR)
(SETTLING)
DISSOLVED
PARTICULATE

Figure 50. Processes influencing the fate of metals in rivers (Mills et al. 1985).

Heavy metals in the aquatic environment can form soluble complexes with organic and inorganic ligands, sorb onto organic and inorganic particulates, and precipitate or dissolve (Figure 51). Geochemical models such as MINTEQ (Felmy et al., 1984) can be used to predict metal speciation for a set of chemical conditions. TOXIWASP lumps all soluble complexes with the free ion to give the dissolved metal concentration. Precipitated metal is lumped with all sorbed species to give particulate "sorbed" metal concentration. A spatially variable lumped partition coefficient K_p describes the two phases. There is no general consistency in reported K_p values for particular metals in the natural environment, so site-specific values should be used when possible. Table 15 summarizes K_p values reported in Delos et al. (1984) for eight metals. These values are generally high, and are provided as a starting

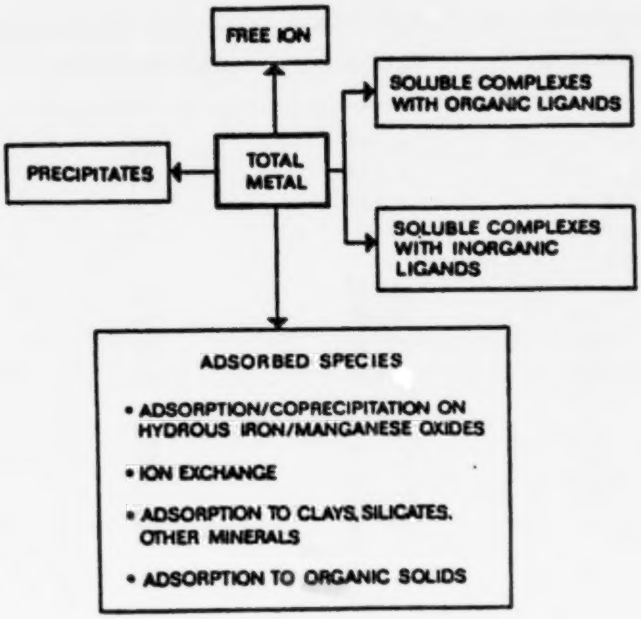

FREE ION
SOLUBLE COMPLEXES WITH ORGANIC LIGANDS
PRECIPITATES
TOTAL METAL
SOLUBLE COMPLEXES WITH INORGANIC LIGANDS
ADSORBED SPECIES
• ADSORPTION/COPRECIPITATION ON HYDROUS IRON/MANGANESE OXIDES
• ION EXCHANGE
• ADSORPTION TO CLAYS, SILICATES, OTHER MINERALS
• ADSORPTION TO ORGANIC SOLIDS

Figure 51. Speciation of metals in aquatic environment (Felmy et al. 1984).

point for the user. Spatially-variable K_p values can be input to TOXIWASP using parameter OCS(ISEG). Constant KOC should be set to 1.0.

1.5.5 Summary of Data Requirements

TOXIWASP adds several specific transport and transformation processes to the basic WASP mass transport equations. These additional processes require the specification of several environmental parameters, chemical constants, and environmental time functions, which were discussed in the preceding sections. This section provides a summary.

The environmental data required for a chemical simulation depend upon which transformation processes are important. Table 16 gives the environmental properties influencing each process in TOXIWASP,and a range of expected values. For a series of simulations involving many compounds, approximate values for all environmental properties should be specified. For those processes found to be most important, better estimates of the relevant environmental properties can be provided in a second round of simulations.

TABLE 15. SPECIATION OF PRIORITY METALS BETWEEN DISSOLVED AND ADSORBED PHASES AS A FUNCTION OF SUSPENDED SOLIDS CONCENTRATIONS IN STREAMS

Metal	SS(mg/L)	K_p(l/kg)	%Dissolved	%Adsorbed
Arsenic	1	5.10^5	70	30
	10	9.10^4	50	50
	100	2.10^4	30	70
	1000	3.10^3	24	76
Cadmium	1	4.10^6	20	80
	10	3.10^5	25	75
	100	2.10^4	30	70
	1000	2.10^3	40	60
Chromium	1	3.10^6	25	75
	10	4.10^5	20	80
	100	5.10^4	17	83
	1000	5.10^3	15	85
Copper	1	1.10^6	50	50
	10	2.10^5	30	70
	100	3.10^4	25	75
	1000	6.10^3	14	86
Lead	1	3.10^5	75	25
	10	2.10^5	30	70
	100	1.10^5	10	90
	1000	9.10^4	1	99
Mercury	1	3.10^6	25	75
	10	2.10^5	30	70
	100	2.10^4	30	70
	1000	1.10^3	45	55
Nickel	1	5.10^5	70	30
	10	1.10^5	50	50
	100	4.10^4	20	80
	1000	9.10^3	10	90
Zinc	1	1.10^6	40	60
	10	2.10^5	30	70
	100	$t.10^4$	17	83
	1000	1.10^4	10	90

TABLE 16. ENVIRONMENTAL PROPERTIES AFFECTING INTERPHASE TRANSPORT AND TRANSFORMATION PROCESSES

Environmental Property (1)	Input Value (2)	Environmental Process K_D (3)	K_S (4)	K_V (5)	K_H (6)	K_O (7)	K_P (8)	K_B (9)
Sediment Concentrations:								
Suspended, in mg/L	5-500	X	X					
Benthic, in kg/L	1.2-1.7	X	X					
Organic Carbon Fraction:								
Suspended Sediment	.01-.10	X	X					
Benthic Sediment	.01-.10	X	X					
Sediment Settling Velocity, in m/day: clays	0-0.3		X					
fine silts	0.1-10							
Bed Sediment Resuspension Velocity, in cm/yr	0-50		X					
Pore Water Diffusion, in cm^2/sec	10^{-5}-10^{-6}		X					
Benthos Mixing Factor	0-1		X					
Surficial Sediment Depth, in cm	0.1-10		X					
Water Column Depth, in m	0.5-100		X	X			X	
Water Column Temperature, in °C	4-30			X	X	X	X	X
Average Water Velocity, in m/sec	0-2			X				
Wind Speed at 10 cm, in m/sec	0-20			X				
pH and pOH, Standard Units	5-9				X			
Concentration of Oxidants, in moles/L	10^{-9}-10^{-12}					X		
Surface Light Intensity, in Langleys/day	300-700						X	
Cloud Cover, tenths of sky	0-10						X	
Light Extinction Coefficient, in per meter	.1-5						X	
Active Bacterial Populations:								
Suspended, in cells/ml	10^3-10^6							X
Benthic, in cells/100g	10^3-10^6							X

(3) Sorption; (4) Benthos-Water Column Exchange; (5) Volatilization; (6) Hydrolysis; (7) Oxidation; (8) Photolysis; (9) Bacterial Degradation

The chemical properties of each compound control that transformation processes are important in a particular environment. Table 17 summarizes chemical properties influencing each process in TOXIWASP. Although the model allows specification of different rates for the dissolved, sorbed, and biosorbed chemical phases, such data are not generally available. Measured rate constants are often assigned to the dissolved chemical phase. The model also allows specification of temperature correction parameters for each process. Such data are often difficult to find without special studies, and need not be input except for very hot or cold conditions, or where seasonal variability is being studied.

Time variable functions can be used to study diurnal or seasonal effects on pollutant behavior. The five time-variable environmental forcing functions are summarized in Table 18. As shown, some of these time functions are multiplied by spatially variable parameters within TOXIWASP to produce time- and spatially-variable environmental conditions.

Although the amount and variety of data potentially used by TOXIWASP is large, data requirements for any particular simulation can be quite small. Usually only sorption and one or two transformation processes will significantly affect a particular chemical. To simulate the transport of many soluble compounds in the water column, even sorption can often be disregarded. Indeed, for empirical studies, all chemical constants, time functions, and environmental parameters can be ignored except the user-specified transformation rate constant TOTKG(ISEG) and, if desired, the partition coefficient-organic fraction pair of KOC and OCS(ISEG). Thus, TOXIWASP can be used as a first-order water pollutant model to conduct standard simulations of dye tracers, salinity intrusion, or coliform die-off. What is gained by the second-order process functions and resulting input data burden is the ability to extrapolate more confidently to future conditions. The user must determine the optimum amount of empirical calibration and process specification for each application.

TABLE 17. BASIC CHEMICAL PROPERTIES AFFECTING INTERPHASE TRANSPORT AND TRANSFORMATION PROCESSES

Variable Name	Chemical Property	Units
GENERAL		
MWTG	Molecular weight	g/mole
SOLG	Solubility	mg/L
SORPTION		
KOW	Octanol-water partition coefficient	L_w/L_o
KOC	Organic carbon partition coefficient	L_w/kg_s
VOLATILIZATION		
HENRYG	Henry's Law constant	m^3-atm/mole
VAPRG	Vapor pressure	torr
KVOG	Liquid phase volatilization/reaeration ratio	--
HYDROLYSIS		
KAHG(I)	Acid-catalysis rate constant for phase I	L/mole-hr
KBHG(I)	Base-catalysis rate constant for phase I	L/mole-hr
KNHG(I)	Neutral rate constant for phase I	hr^{-1}
OXIDATION		
KOXG(I)	Second order rate constant for phase I	L/mole-hr
PHOTOLYSIS		
KDPG	Near surface, reference rate constant	hr^{-1}
QUANTG(I)	Reaction yield for phase I	--
BIODEGRADATION		
KBACWG(I)	Second order rate constant in water for phase I	ml/cell-hr
KBACSG(I)	Second order rate constant in benthos for phase I	ml/cell-hr

TABLE 18. TIME VARIABLE ENVIRONMENTAL FORCING FUNCTIONS

	Time Function		Parameter		Environmental Property
	TEMPN	x	TEMPM(ISEG)	=	Water temperature (x,t)
	(Unitless)		(°C)		°C
or	(°C)		(unitless)		°C
	WINDN	x	WINDG(ISEG)	=	Wind speed at 10 cm above surface (x,t)
	(unitless)		(m/sec)		(m/sec)
or	(m/sec)		(unitless)		(m/sec)
	PHN	x	PHG(ISEG)	=	Average pH (x,t)
	(unitless)		(log activity)		(log activity)
or	(log activity)		(unitless)		(log activity)
	POHN	x	POHG(ISEG)	=	Average pOH (x,t)
	(unitless)		(log activity)		(log activity)
or	(log activity)		(unitless)		(log activity)
	LIGHTN		--	=	Average normalized light intensity at water surface (t)
	(unitless)				(unitless)

SECTION 2

WASP3 USER'S MANUAL

2.1 OVERVIEW

To run the WASP3 or DYNHYD3 models, an input data set must be specified. These data sets are catalogued into input data groups (formerly "card groups") and are read into the programs in batch mode. For convenience, the data sets are separated according to subject matter.

Each card group contains several "records" or lines. Records are usually one 80-space line, but in a few instances a record will constitute as many lines as needed to complete the data group. Records are always input sequentially and each record begins on a new line. Do not skip lines between records unless a "blank" record is specifically instructed. Likewise, do not enter blank lines between data groups; the models simply read from one line to the next.

The introduction in each section gives an overview for each of the data group's subject matter. The data group descriptions give detailed information of all records and detailed definitions for all variables in that group. The data group tables provide quick reference to record structure, variable format, and definition. The variable definition section supplies an alphabetical listing with definitions for all variables (of that particular model).

This manual consists of a section for each of four models--the hydrodynamic model, the basic water quality model, the eutrophication model, and the toxics model. Within each section, there is an introduction, description of data groups, data group tables, and variable definitions. For the basic water quality section, the variable definitions are provided for the common blocks only. Within the eutrophication and toxics sections, only those data group descriptions specifically pertaining to EUTRWASP or TOXIWASP are provided.

2.2 THE HYDRODYNAMIC MODEL

2.2.1 Introduction

This section describes the input required to run the DYNHYD3 hydrodynamics program. To arrange the input into a logical format, the data are divided into eight groups:

A - Simulation Control
B - Printout Control
C - Hydraulic Summary
D - Junction Data
E - Channel Data
F - Inflow Data
G - Seaward Boundary Data
H - Wind Data

The following is a brief explanation of each data group.

Data Group A consists of preliminary data, such as network parameters (number of channels, number of junctions), simulation time step, and the beginning and ending day of simulation.

Data Group B allows the user to specify printing options.

Data Group C is responsible for the storage of flows and volumes. The stored file created by this data group can be used as an input data set for the water quality model.

Data Group D describes the model network and initial conditions at each junction.

Data Group E describes the model network and initial conditions at each channel.

Data Group F lists all inflows into the model system. Flows may be constant or variable. Inflows are considered to be negative, and outflows are positive.

Data Group G describes the seaward boundaries. The maximum number of seaward boundaries has been set to five, but can be respecified by the user. There are two types of tidal inputs: average tide, and variable tide. The average tide is a smooth, repetitive curve that fits the equation:

$$\begin{aligned} \text{Head} = A_1 + {} & A_2 \sin(\omega t) \\ & A_3 \sin(2\omega t) \\ & A_4 \sin(3\omega t) \\ & A_5 \cos(\omega t) \\ & A_6 \cos(2\omega t) \\ & A_7 \cos(3\omega t) \end{aligned} \tag{160}$$

The variable tide is a 1/2 sine wave that has highs and lows as specified by the data set.

Data Group G has three options for defining the tidal cycle. Option 1, the user specifies the coefficients in equation 160 for an average tide. Option 2, the user specifies data and the model calculates the coefficients in equation 160 which define the average tide. Option 3, the user specifies the highs and lows of a variable tide and the model fits a half sine curve through the points.

Data Group H lists wind speeds and directions.

2.2.2 DYNHYD3 Data Group Descriptions

2.2.2.1 DATA GROUP A: Simulation Control--

VARIABLES

Records 1, 2--Model Identification

ALPHA(J) = alphanumeric characters to identify the system, date and run number.

Record 3--Data Group Identification

HEADER = alphanumeric characters to identify the data group, "PROGRAM CONTROL DATA."

Record 4--Simulation Control Data

NJ = number of junctions in the model network.

NC = number of channels in the model network.

NCYC = total number of time steps for execution (number of cycles). If equal to zero, the model will compute NCYC internally (cycles).

DELT = time interval used in execution (sec).

ICRD = file containing the initial conditions for junctions and channels. If equal to 0 or 5, data set is read. If equal to 8, a file 8, previously created by subroutine RESTART, is read.

ZDAY = beginning day of simulation (day).

ZHR = beginning hour of simulation (hr).

ZMIN = beginning minute of simulation (min).

EDAY = ending day of simulation (day).

EHR = ending hour of simulation (hr).

EMIN = ending minute of simulation (min).

ALPHA(1), ALPHA(2), and HEADER assist the user in maintaining a log of computer simulations, but are not actually used by the DYNHYD3 program.

ORGANIZATION OF RECORDS

Each record in Data Group A is input once; therefore, Data Group A consists of 4 lines of data. Data Group B starts on the 5th line (no blank line).

2.2.2.2 DATA GROUP B: Printout Control--

VARIABLES

Record 1--Data Group Identification

HEADER = alphanumeric characters to identify the data group, "PRINTOUT CONTROL DATA."

Record 2--Output Control Information

FPRINT = time for printout to begin (hr).

PINTVL = time interval between printouts (hr).

NOPRT = number of junctions for which printouts (results) are desired, can be 1 through NJ.

Record 3--List of Junctions

JPRT(I) = junction number for results to be printed.

There will be NOPRT entries in Record 3 (I = 1 to NOPRT).

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once. Record 3 may contain several lines depending upon NOPRT. One line may contain up to 16 entries. Therefore, if NOPRT is equal to 1-16, then Record 3 will consist of 1 line. If NOPRT is equal to 17-32, then Record 3 will consist of 2 lines, etc. The total number of lines for Data Group B equals 2 + (1 + INT((NOPRT-1)/16))).

2.2.2.3 DATA GROUP C: Hydraulic Summary--

VARIABLES

Record 1--Data Group Identification

HEADER = alphanumeric characters to identify the data group "Summary Control Data."

Record 2--Summary Control Data

SUMRY = option number that controls how the hydrodynamic scratch file (file 2) is processed to create a permanent summary file (file 4) for the water quality model to read. If equal to zero, then no summary file will be created. If equal to 1, an unformatted file will be created, which is unlegible, but quicker and saves space. If equal to 2, a formatted file will be created which is legible.

TDAY = day to begin storing parameters to file (day).

THR = hour to begin storing parameters to file (hr).

TMIN = minute to begin storing parameters to file (min).

NODYN = number of hydraulic time steps per quality time steps desired.

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once. Therefore, Data Group C consists of two lines.

2.2.2.4 DATA GROUP D: Junction Data--

VARIABLES

Record 1--Data Group Identification

HEADER = alphanumeric characters to identify the data group, "JUNCTION DATA."

Record 2--Junction Parameters

JJ = junction number.

Y(J) = initial head (or surface elevation) in reference to a horizontal model datum, at junction JJ (ft).

SURF(J) = surface area at junction JJ (ft^2).

BELEV(J) = bottom elevation above (or below) the horizontal datum plane (usually taken to be mean sea level) (ft).

NCHAN(J,I)= channel number entering junction JJ. Maximum number of channels entering any one junction is five (I = 1 - 5). Start list with lowest channel number.

ORGANIZATION OF RECORDS

Record 1 is entered once in Data Group D. Record 2 is entered NJ times (NJ = number of junctions). One line is used for each junction. Therefore, Data Group D consists of 1 + NJ lines.

2.2.2.5 DATA GROUP E: Channel Data--

VARIABLES

Record 1--Data Group Identification

HEADER = alphanumeric characters to identify the data group, "CHANNEL DATA."

Record 2--Channel Parameters

NN = channel number.

CLEN(N) = length of channel NN (ft).

B(N) = width of channel NN (ft).

R(N) = hydraulic radius or depth of channel NN (ft).

CDIR(N) = channel direction, or angle in degrees measured from true north. The channel direction points in the direction of positive flow, from the higher junction number to the lower junction number (degrees)

CN(N) = Manning roughness coefficient for channel NN (sec . $m^{-1/3}$). Ranges from 0.01 to 0.08.

V(N) = the initial mean velocity in channel NN, ft/sec.

NJUNC(N,1)= the connecting junction at the lower end of channel NN.

NJUNC(N,2)= the connecting junction at the higher end of channel NN.

A channel may only connect two junctions. Therefore, only NJUNC(N,1) and NJUNC(N,2) exists.

ORGANIZATION OF RECORDS

Record 1 is entered only once in Data Group E. Record 2 is entered NC times (NC = number of channels). One line is used for each channel. Therefore, Data Group E consists of 1 + NC lines.

2.2.2.6 DATA GROUP F: Inflow Data--

VARIABLES

Record 1--Data Group Identification

HEADER = alphanumeric characters to identify the data group and type of inflows, "CONSTANT INFLOW DATA."

Record 2--Constant Inflow Number

NCFLOW = the number of constant inflows that will be read.

Record 3--Constant Inflow Data

JRCF(I) = junction that will be receiving the following inflow.

CFLOW(I) = the value of the constant inflow into junction JRCF(I) (ft^3/sec). Value will be negative for inflow, positive for outflow.

Record 4--Data Group Identification

HEADER = alphanumeric characters to identify the type of inflows, "VARIABLE INFLOW DATA."

Record 5--Variable Inflow Number

NVFLOW = the number of variable inflows that will be read

Record 6--Variable Inflow Breaks

JRVF(I) = junction that will be receiving the following variable inflows.

NINCR(I) = number of data points (breaks) for variable inflow into junction JRVF(I).

Record 7--Variable Inflow Data

DAY(K) = day of VFLOW(I,K) (day).

HR(K) = hour of VFLOW(I,K) (hr).

MIN(K) = minute of VFLOW(I,K) (min).

VFLOW(I,K)= value of the variable flow corresponding to DAY(K), HR(K), and MIN(K) (ft^3/sec). Value will be negative for inflow, positive for outflow.

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in Data Group F. Record 3 is entered NCFLOW times with one junction number and one flow per line. Records 4 and 5 are entered once in Data Group F. Record 6 is entered NVFLOW times, but not consecutively. Record 6 should be entered (one junction, one number of breaks), then Record 7 with 4 flows per line until NINCR(I) flows have been entered. Then Record 6 entered again followed by Record 7. The number of lines for Data Group F is equal to

4 + NCFLOW + NVFLOW (1 + INT((NOPRT-1)/16))

2.2.2.7 DATA GROUP G: Seaward Boundary Data--

VARIABLES

Record 1--Data Group Identification

HEADER = alphanumeric characters to identify the data group, "SEAWARD BOUNDARY DATA."

Record 2--Seaward Boundary Number

NSEA = number of seaward boundaries on model network.

If NSEA >0, proceed to Record 3. If NSEA = 0, go to Data Group H.

Record 3--Seaward Boundary Parameters

JJ = junction number receiving the tidal input.

NDATA = number of data points (or breaks) to calculate the coefficients to the curve:

$$\begin{aligned}\text{Head} = A1(J,1) &+ A2(J,2)\ \sin(\omega t)\\ &+ A3(J,3)\ \sin(2\omega t)\\ &+ A4(J,4)\ \sin(3\omega t)\\ &+ A5(J,5)\ \cos(\omega t)\\ &+ A6(J,6)\ \cos(2\omega t)\\ &+ A7(J,7)\ \cos(3\omega t)\end{aligned}$$

NTV(J) = number of data points (breaks) used to describe the variable tide.

MAXIT = maximum number of iterations allowed to calculate average tide.

MAXRES = maximum error allowed in calculation of average tide (calculates coefficients to describe tidal cycle).

TSHIFT = allows tidal cycle to be shifted on the time scale. Therefore, if all data have been entered and error of 6.5 hours has been made in time scale, one can enter 6.5 for TSHIFT (hr). Usually equal to zero.

PSHIFT = allows tidal cycle to be shifted on the phase angle scale (radians). Usually equal to zero.

YSCALE = scale factor for observed heads, B(HEAD) = B(HEAD) * YSCALE.

If NTV(J) = 0 and NDATA >0, use Records 4 and 5 => calculates coefficients for average tide.

If NTV(J) = 0 and NDATA = 0, use Records 4 and 6 => coefficients for average tide are given.

If NTV(J) >), use Record 5 => variable tide is calculated.

Record 4--Tidal Parameters

PERIOD(J) = tidal period (hr).

TSTART(J) = starting time for tidal input (hr).

Record 5--Tidal Data

DAY(I) = day corresponding to BHEAD(I) (day).

HR(I) = hour corresponding to BHEAD(I) (hr).

MIN(I) = minute corresponding to BHEAD(I) (min).

BHEAD(I) = tidal elevation (head) at time DAY(I), HR(I), and MIN(I) (ft).

Record 6--Coefficients

A1(J,1) = 1st Coefficient.

A1(J,2) = 2nd Coefficient

A1(J,3) = 3rd Coefficient.

A1(J,4) = 4th Coefficient.

A1(J,5) = 5th Coefficient.

A1(J,6) = 6th Coefficient.

A1(J,7) = 7th Coefficient.

These coefficients describe the curve with the following equation:

$$\begin{aligned} \text{Head} = A1(J,1) &+ A2(J,2)\sin(\omega t) \\ &+ A3(J,3)\sin(2\omega t) \\ &+ A4(J,4)\sin(3\omega t) \\ &+ A5(J,5)\cos(\omega t) \\ &+ A6(J,6)\cos(2\omega t) \\ &+ A7(J,7)\cos(3\omega t) \end{aligned}$$

ORGANIZATION OF RECORDS

As discussed in Section 2.2.1, three options for describing the tidal cycle exists: 1) give coefficients for average tide, 2) calculate coefficients for average tide, or 3) give highs and lows for variable tide. For all three options, records 1, 2, and 3 are entered once. For Option 1 (NTV=0, NDATA=0 => records 4 and 6): Record 4 and Record 6 are entered once.

For Option 2 (NTV=0, NDATA>0 => records 4 and 5): Record 4 is entered once, and Record 5 is entered as many times as needed with 4 tidal elevations on each line.

For Option 3 (NTV >0, NDATA = 0 => Record 5): Record 5 is entered as many times as needed with 4 tidal elevations on each line.

The total number of lines is 2 + a set for each of NSEA tidal boundaries.

For Option 1, the set will include 1 + 1 + 1 + INT((NDATA-1)/4).

For Option 2, the set will include 1 + 1 + 1.

For Option 3, the set will include 1 + 1 + INT((NTV-1)/4).

.2.2.8 DATA GROUP H: Wind Data--

VARIABLES

Record 1--Data Group Identification

HEADER = alphanumeric characters to identify the data group, "WIND DATA."

Record 2--Wind Data Number

NOBSW = number of wind data points (or breaks)

Record 3--Wind Data

DAY(K) = day corresponding to the following wind speed and wind direction (day).

HR(K) = hour corresponding to the following wind speed and wind direction (hr).

MIN(K) = minute corresponding to the following wind speed and wind direction (min).

WINDS(K) = wind speed measured at a distance of 10 meters above the water system (ft/sec).

WDIR(K) = wind direction measured at a distance of 10 meters above the water system. Must be measured from True North (degrees).

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once for Data Group H. Record 3 is entered as many times as needed with 4 wind speeds on each line. The total number of lines in Data Group H is equal to 2 + (1 + INT((NOBSW-1)/4).

2.2.3 DYNHYD3 Data Group Tables

DATA GROUP A: Simulation Control

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1,2	ALPHA(J)	1-80	20A4	Two records to identify the system, date, and run number.
3	HEADER	1-80	20A4	Title: "PROGRAM CONTROL DATA"
4	NJ	1-5	I5	Number of junctions in network.
	NC	6-10	I5	Number of channels in network.
	NCYC	11-15	I5	Total number of time steps.
	DELT	16-20	F5.0	Time interval used in solution (sec).
	ICRD	21-25	I5	File containing initial conditions.
	ZDAY	26-30	F5.0	Beginning day of simulation (day).
	ZHR	32-33	1X,F2.0	Beg. hour of simulation (hr).
	ZMIN	34-35	F2.0	Beg. minute of simulation (min).
	EDAY	36-40	F5.0	Final day of simulation (day).
	EHR	42-43	1X,F2.0	Final hour of simulation (hr).
	EMIN	44-45	F2.0	Final minute of simulation (min).

DATA GROUP B: Printout Control

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1	HEADER	1-80	20A4	Title: "PRINTOUT CONTROL DATA"
2	FPRINT	1-10	F10.0	Time used for first printout (hr).
	PINTVL	11-20	F10.0	Time interval between printout (hr).
	NOPRT	21-25	I5	Number of junctions to be printed.
3	JPRT(1)	1-5	I5	First junction number for results to be printed.
	JPRT(2)	6-10	I5	Second junction number for results to be printed.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	.	76-80	.	(Use as many 80-space lines as needed to enter NOPRT values)
	JPRT(NOPRT)	1-5	I5	
		.		
		.		
		.		

DATA GROUP C: Hydraulic Summary

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1	HEADER	1-80	20A4	Title - "Summary Control Data"
2	SUMRY	1-5	I5	= 0, 1, or 2. See definition.
	TDAY	6-10	F5.0	Day to begin storing parameters (day).
	THR	12-13	1X,F2.0	Hour to begin storing parameters (hr).
	TMIN	14-15	F2.0	Minute to begin storing parameters (min).
	NODYN	16-20	I5	No. time steps/ quality time steps.

DATA GROUP D: Junction Data

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1	HEADER	1-80	20A4	Title: "JUNCTION DATA"
				J = 1
2	JJ	1-5	I5	Junction number.
	Y(J)	6-15	F10.0	Head at junction J (ft).
	SURF(J)	16-25	F10.0	Surface area at junction J (ft^2).
	BELEV(J)	26-35	F10.0	Bottom elevation at junction J (ft).
	NCHAN(J,1)	36-40	I5	First channel entering junction J.
	NCHAN(J,2)	41-45	I5	Second channel entering junction J.
	NCHAN(J,3)	46-50	I5	.
	NCHAN(J,4)	51-55	I5	.
	NCHAN(J,5)	56-60	I5	Fifth channel entering junction J.
	. . .	. . .	. . .	. . .
NJ				J = NJ
	JJ			Use as many lines as needed,
	Y(J)	.	.	repeating the above format, until
	SURF(J)	.	.	NJ lines have been entered.
	BELEV(J)	.	.	
	NCHAN(J,1)			
	NCHAN(J,2)			
	NCHAN(J,5)			

DATA GROUP E: Channel Data

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1	HEADER	1-80	20A4	Title: "CHANNEL DATA"
				N = 1
2	NN	1-5	I5	Channel number.
	CLEN(N)	6-15	F10.0	Length of channel N (ft).
	B(N)	16-25	F10.0	Width of channel N (ft).
	R(N)	26-35	F10.0	Hydraulic radius (or depth) (ft).
	CDIR(N)	36-45	F10.0	Channel direction (degrees).
	CN(N)	46-55	F10.0	Manning coeff. for channel N.
	V(N)	56-65	F10.0	Mean velocity in channel N (ft/sec).
	NJUNC(N,1)	66-70	I5	Lower jnct. number entering channel.
	NJUNC(N,2)	71-75	I5	Higher jnct. no. entering channel.
	.	.	.	.
	.	.	.	.
	.	.	.	.
NC				N = NC
	NN			Use as many lines as needed,
	CLEN(N)	.	.	repeating the above format, until
	B(N)(J)	.	.	NJ lines have been entered.
	R(N)V(J)	.	.	
	CDIR(N),1)			
	CN(N)(J,2)			
	V(N)(J,5)			
	NJUNC(N,1)			
	NJUNC(N,2)			

DATA GROUP F: Inflow Data

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1	HEADER	1-80	20A4	Title: "CONSTANT INFLOW DATA"
2	NCFLOW	1-5	I5	Number of constant flow inputs.
3	JRCF(I)	1-10	I10	Junction receiving constant flow I.
	CFLOW(I)	11-20	F10.0	Cnst. inflow (-) or outflow (+) I (ft^3/sec). (One line per flow)
4	HEADER	4-80	20A4	Title: "VARIABLE INFLOW DATA"
5	NVFLOW	1-5	I5	Number of variable flow inputs.

Continued

DATA GROUP F: Inflow Data (Continued)

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
6	JRVF(I)	1-10	I10	Jnct. receiving variable flow I.
	NINCR(I)	11-20	I10	Number of data points for variable inflow in junction I.
7	DAY(K)	1-5	F5.0	Day corresponding to VFLOW(1,1) (day).
	HR(K)	7-8	1X,F2.0	Hour corresponding to VFLOW(1,1) (hr).
	MIN(K)	9-10	F2.0	Minute corresponding to VFLOW(1,1) (min).
	VFLOW(I,K)	11-20	F10.0	Variable flow (ft^3/sec).
	DAY(K)	21-25	.	K=2
	HR(K)	27-28	.	
	MIN(K)	29-30	.	
	VFLOW(I,K)	31-40		
	DAY(K)	41-45	.	K=3
	HR(K)	47-48	.	
	MIN(K)	49-50	.	
	VFLOW(I,K)	51-60		
	DAY(K)	61-65	.	K=4
	HR(K)	67-68	.	
	MIN(K)	69-70	.	
	VFLOW(I,K)	71-80		
	.	1-5	.	(Uses as many 80-space lines as needed to input NFLOW sets of data, repeating the format above).
	.	7-8	.	
	.	9-10	.	
		11-20		
	DAY(K)	21-25	F5.0	K=NVFLOW
	HR(K)	27-28	F2.0	
	MIN(K)	29-30	F2.0	
	VFLOW(I,K)	31-40	F10.0	

DATA GROUP G: Seaward Boundary Data

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1	HEADER	1-80	20A4	Title: "SEAWARD BOUNDARY DATA"
2	NSEA	1-5	I5	Number of seaward boundaries
	If NSEA > 0, proceed to record 3. If NSEA = 0, go to Data Group H.			
3	JJ	1-5	I5	Junction number
	NDATA	6-10	I5	No. data pts. to find average tide.
	NTV(J)	11-15	I5	No. data pts. for variable tide.
	MAXIT	16-20	I5	Max. iters. to calculate ave. tide.
	MAXRES	21-25	I5	Max. error allowed in calculation.
	TSHIFT	26-30	F5.0	Shifts time scale (hr).
	PSHIFT	31-35	F5.0	Shifts phase angle (radians).
	YSCALE	36-40	F5.0	Scale factor for observed B(HEAD).
(Option 1) If NTV(J) = 0 and NDATA = 0, use records 4 and 5. (Option 2) If NTV(J) = 0 and NDATA > 0, use records 4 and 6. (Option 3) If NTV(J) > 0, use record 5.				
4	PERIOD(J)	1-10	F10.0	Period of tidal input (hr).
	TSTART(J)	11-20	F10.0	Starting time for tidal input (hr).
				I=1
5	DAY(I)	1-5	F5.0	Day corresponding to BHEAD(1) (day).
	HR(I)	6-8	1X,F2.0	Hour corresponding to BHEAD(1) (hr).
	MIN(I)	9-10	F2.0	Minute corresponding the BHEAD(1) (min).
	BHEAD(I)	11-20	F10.0	Tidal elevation (feet)
	DAY(I)	21-25	F5.0	I=2
	HR(I)	26-28	1X,F2.0	
	MIN(I)	29-30	F2.0	
	BHEAD(I)	31-40	F10.0	
	.	.	.	I=3
	.	.	.	
	.	.	.	
	DAY(I)	61-65	F5.0	I=4
	HR(I)	67-68	1X,F2.0	
	MIN(I)	69-70	F2.0	
	BHEAD(I)	71-80	F10.0	
	.	.	.	Use as many lines as needed, repeating the above format, until NDATA sets (of time and head) are entered.
	.	.	.	
	.	.	.	
	DAY(I)	.	.	I=NDATA
	HR(I)	.	.	
	MIN(I)			
	BHEAD(I)			

DATA GROUP G: Seaward Boundry Data (Continued)

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
6	A1(J,1)	1-10	F10.0	Head = A1(J,1)
	A1(J,2)	11-20	F10.0	$+ A_2(J,2) \sin(\omega t)$
	A1(J,3)	21-30	F10.0	$+ A_3(J,3) \sin(2\omega t)$
	A1(J,4)	31-40	F10.0	$+ A_4(J,4) \sin(3\omega t)$
	A1(J,5)	41-50	F10.0	$+ A_5(J,5) \cos(\omega t)$
	A1(J,6)	51-60	F10.0	$+ A_6(J,6) \cos(2\omega t)$
	A1(J,7)	61-70	F10.0	$+ A_7(J,7) \cos(3\omega t)$

DATA GROUP H: Wind Data

RECORD	VARIABLE	COLUMN	FORMAT	SHORT DEFINITION
1	HEADER	1-80	20A4	Title: "WIND DATA"
2	NOBSW	1-5	I5	Number of data points.
				K=1
3	DAY(K)	1-5	F5.0	Day corresponding to WINDS(K) (day).
	HR(K)	7-8	1X,F2.0	Hour corresponding to WINDS(K) (hr).
	MIN(K)	9-10	F2.0	Min corresponding to WIND(K) (min).
	WINDS(K)	11-15	F5.0	Wind speed (ft/sec).
	WDIR(K)	16-20	F5.0	Wind direction (degrees).
	.	.	.	
	.	.	.	
	.	.	.	
	.	.	.	
	DAY(K)	61-65	F5.0	K=4
	HR(K)	67-68	1X,F2.0	
	MIN(K)	69-70	F2.0	
	WINDS(K)	71-75	F5.0	
	WDIR(K)	76-80	F5.0	
	.	.	.	Repeat as necessary, using above
	.	.	.	format, until NOBSW groups of DAY,
	.	.	.	HR, MIN are entered.
	DAY(K)	1-5	F5.0	K=NOBSW
	HR(K)	7-8	1X,F2.0	
	MIN(K)	9-10	F2.0	
	WINDS(K)	11-15	F5.0	
	WDIR(K)	16-20	F5.0	

2.2.4 DYNHYD3 Variable Definitions

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
AK(N)	DYNHY2 RUNKUT	Friction coefficient for channel N.	$ft^{1/3}$
*ALPHA(I)	DYNHYD	Alphanumeric identifier to be printed as part of output, (I = 1,80)	unitless
AREA(N)	DYNHYD RUNKUT RESTRT SUMRY1,2	Cross-sectional area of channel N, corresponding to junction heads specified at each end of the channel.	ft^2
AREAT	RUNKUT	Cross-sectional area of channel N during half time step.	ft^2
AVGD	DYNHYD	Average depth of the channel used to cal culate average volume of connecting junction.	ft
AVGDEP	SUMRY1,2	Average channel depth; calculated by subroutine MEAN.	ft
AVGQIN	SUMRY1,2	Average flow in channel.	ft^3/sec
AVGVEL	SUMRY1,2	Average velocity in channel.	ft/sec
*A1(J,I)	SEAWRD	Value of the I-th tidal coefficient (I = 1,7) for seaward boundary J, obtained from program REGAN.	unitless
*BELEV(J)	DYNHYD	Bottom elevation above (or below) the horizontal datum plane (usually) taken to be mean sea level).	ft
*BHEAD(J,L)	SEAWRD REGAN RUNKUT	Head at junction J, at time DAY(L), HR(L), MIN(L). Used for variable tides.	ft
*B(N)	DYNHYD RUNKUT RESTRT SUMRY1,2	Width of channel N.	ft

*Denotes input variables

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
BTIME(J,L)	SEAWRD RUNKUT	Time in seconds; calculated from DAY(L), HR(L), and MIN(L) at junction J. Corresponds to variable head (BHEAD(J, K)).	sec
BTMP	DYNHYD	Accumulative bottom elevation above (or below) the horizontal datum plane (usually taken to be mean sea level).	ft
*CDIR(N)	DYNHYD WIND	Channel direction, or angle in degrees from the north. The channel direction points in the direction of positive flow, from the higher junction number to the lower junction number.	degrees
*CFLOW(I)	DYNHYD SUMRY1,2	Constant inflow (negative) or outflow (positive) I.	ft^3/ sec
*CLEN(N)	DYNHYD RUNKUT RESTRT SUMRY1,2	Length of channel N.	ft
*CN(N)	DYNHYD RESTRT	Manning roughness coefficient for channel N.	sec/ $m^{1/3}$
CQIN(J)	DYNHYD RUNKUT	Constant inflow for junction J.	ft^3/ sec
CVOL	DYNHYD	Channel volume (area * depth).	ft^3
*DAY(K)	DYNHYD WIND	Day of tidal data point.	days
DEL	REGAN	Residual error for calculating	unitless
*DELT	DYNHYD DEAWRD WIND RUNKUT RESTRT SUMRY1,2	Time interval used in solution.	sec

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
DELTQ	SUMRY1,2	Time step for the quality program (DELTQ = DELT * NODYN/3600).	hr
DEP(N,1)	SUMRY1,2	Hydraulic radius of channel N.	ft
DIFF	REGAN	Difference in actual and predicted value of tidal height.	ft
DT	DYNHYD SEAWRD RUNKUT	Full time interval.	sec
DT2	DYNHYD SEAWRD RUNKUT	1/2 time interval.	sec
DTIME(J)	SEAWRD RUNKUT	Range between last variable tide data point and first variable tide data point.	sec
DVDT	RUNKUT	Total acceleration term.	ft/ sec^2
DVDT1	RUNKUT	Momentum acceleration term.	ft/ sec^2
DVDT2	RUNKUT	Friction acceleration term.	ft/ sec^2
DVDT3	RUNKUT	Gravity acceleration term.	ft/ sec^2
DVDT4	RUNKUT	Wind acceleration term.	ft/ sec^2
DVDX	RUNKUT	Velocity gradient ($\Delta v/\Delta x$) in a channel.	ft/ sec-ft
DVOL	RUNKUT	Differential junction volume for 1/2 time step.	ft^3
DY	RUNKUT	The average change in channel head over 1/2 time step.	ft
DYDT	RUNKUT	The average rate of change of head in a channel over 1/2 time step.	ft/ sec
DYDX	RUNKUT	The water surface slope over a channel at a 1/2 time step.	ft/ft

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
*EDAY	DYNHYD	Ending day of simulation.	day
*EHR		Ending hour of simulation.	hr
*EMIN		Ending minute of simulation.	min
FLO(N,1)	SUMRY1,2	Flow at channel N.	ft^3/sec
*FPRINT	DYNHYD	Time which the first printout is desired.	hr
FW(N)	WIND RUNKUT	Wind acceleration term.	ft/sec^2
G	DYNHYD	Acceleration due to gravity (32.1739 ft/sec^2).	ft/sec^2
*HEADER	DYNHYD SEAWRD WIND	Alphanumeric identifier for each data group.	unitless
*ICRD	DYNHYD	File containing initial conditions for junctions and channels (defaults to Unit 5).	unitless
INTRVL	DYNHYD	Interval (in cycles) between printouts.	cycles
IPRINT	DYNHYD	Printed output begins at this cycle, and each INTRVL cycle thereafter.	cycles
IREADW	DYNHYD WIND	Switch to read in wind data once.	unitless
ITAPE	DYNHYD SUMRY1,2	Hydraulic parameters are stored on Unit 2 beginning at this cycle.	cycles
IW	WIND	Counter	unitless
*JJ	DYNHYD SEAWRD	Junction number.	junction
*JPRT(I)	DYNHYD	Specified junction for which printout is desired (I = 1, NOPRT).	junction
*JRCF(I)	DYNHYD SUMRY1,2	Junction receiving constant flow I.	junction

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
*JRVF(I)	DYNHYD SUMRY1,2	Junction receiving variable flow I.	junction
*J1-J5	DYNHYD SUMRY1,2	Specified junctions for results to be printed.	junction
KT	RUNKUT	Friction coefficient during full time step.	1/ft
KT2	RUNKUT	Friction coefficient during half time step.	1/ft
LTAPE	DYNHYD SUMRY1,2	Last hydraulic time step written to TAPE	cycles
*MAXIT	SEAWRD REGAN	Maximum number of iterations desired in the run.	unitless
*MAXRES	SEAWRD REGAN	Maximum value of the residual allowed. Will not be exceeded unless the number of iterations reaches MAXIT before the residual reaches MAXRES. A value of 0.0001 is typically used.	unit-
MIN(K)	DYNHYD WIND	Minute for data point.	min
MXCH	SUMRY1,2	Maximum number of rows in matrix transferred to x. Another name is MXROW.	unitless
MXJU	SUMRY1,2	Maximum number of rows in matrix transferred to x. Another name is MXROW.	unitless
MXNR	SUMRY1,2	Maximum number of columns in matrix transferred to x. Another name is MXCOL.	unitless
*NC	DYNHYD WIND RUNKUT SUMRY1,2	Number of channels in model network.	channels
*NCFLOW	DYNHYD SUMRY1,2	Number of constant flow inputs.	unitless
*NCHAN (J,K)	DYNHYD RUNKUT RESTRT SUMRY1,2	Channel number entering junction J. Maximum number of channels entering a junction equals 5 (K=1-5).	channel

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
NCOEFF	REGAN	Number of coefficients used to describe average tide (=7).	unitless
NCOL	MEAN	Number of columns in matrix X. Corresponds to the number of data points. Must be odd if NOPT = 1.	unitless
*NCYC	DYNHYD RESTRT	Total number of time steps (cycles to be executed). If 0, is calculated internally.	
*NDATA	SEAWRD REGAN SUMRY1,2	Number of input data points over a tidal cycle. This information is used to calculate the coefficients describing the tide. Use as many data points as possible.	unitless
NH	DYNHYD REGAN	Lower of the two junction numbers of each end of channel N.	junction
*NINCR(I)	DYNHYD SUMRY1,2	Number of increments in variable flow record I.	unitless
NINL	SEAWRD RUNKUT	Number of seaward boundaries plus one.	unitless
*NJ	DYNHYD RUNKUT SUMRY1,2	Number of junctions in the model network.	junction
*NJUNC (N,K)	DYNHYD RUNKUT SUMRY1,2	K = 1: Lower of the two junction numbers at each end of channel N. K = 2: Higher of the two junction numbers at the end of channel N.	junction
NK	SEAWRD RUNKUT	Number of coefficients used to specify tidal input (= 7).	unitless
NL	DYNHYD RUNKUT	Higher of the two junction numbers at each end of channel N.	junction
*NN	DYNHYD RESTRT	Channel number.	channel
*NOBSW	WIND	Number of wind observations (number of wind data sets).	unitless
*NODYN	DYNHYD SUMRY1,2	Number of hydraulic time steps per quality time step.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
*NOPRT	DYNHYD	Number of junctions for which output is desired.	unit-less
NRSTRT	DYNHYD RESTRT	Time at which SUMRY should start writing flows and heads to tape for water quality simulation. Claculated from day, hr, min.	sec
NS	SEAWRD RUNKUT	NK/2. Number of sine and cosine terms in relationship defining tidal input.	unit-less
*NSEA	SEAWRD RUNKUT	Number of seaward boundaries.	unit-less
NTIDES	SEAWRD	Number of tidal periods in simulation.	periods
*NTV(J)	SEAWRD RUNKUT	Number of variable tide data points. Use only the highs and lows of a tiday cycle, and be sure the first and last are the same.	unit-less
NX	DYNHYD	Number of data points for variable inflows in junction I.	unit-less
NZERO	DYNHYD	NRSTRT plus one.	sec
*N1-N5	DYNHYD	Specified channels for DYNHYD check printout.	channel
*PERIOD(J)	SEAWRD	Tidal period. PERIOD is read in as hours, but transformed to seconds within the program.	hr
*PINTVL	DYNHLYD	Time interval between printouts.	hr
PRED	REGAN	Predicted value of tidal input.	ft
*PSHIFT	SEAWRD REGAN	Variable which shifts the phase angle in the trigonometric relationship (usually = 0).	radians
QCYC(I,K)	DYNHYD SUMRY1,2	Hydrodynamic cycle (time step) at increment K in variable flow record I.	cycles
QINSAV(J)	SUMRY1,2	Inflow into junction J.	ft^3/sec

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
QINS(J,1)	SUMRY1,2	Inflow into junction J.	ft^3/sec
QTIME	DYNHYD	An intermediate variable giving the time in seconds corresponding to a variable flow VFLOW (I,K).	sec
RANGE(J)	SEAWRD	Tidal range at junction J (RANGE(J) = YMAX(J)- YMIN(J).	ft
RESID	REGAN	Residuals.	unitless
*R(N)	DYNHYD RUNKUT SUMRY1,2	Hydraulic radius of channel N, taken as the channel depth.	ft
RT(I)	REGAN	Time of the I^{th} specified data point on the input tide (I = 1, NDATA).	hr
SAREA	DYNHYD	Channel surface area (length * width).	ft^2
SASUM	DYNHYD	Total channel surface area connected to junction J.	ft^2
SUM	REGAN	Coefficients used in describing tidal cycle (= A(K)).	unitless
*SUMRY	DYNHYD SUMRY1	Controls how hydrodynamic file 2 is processed to create a permanent summary file 4. If 0, no file created. If 1, transient conditions are saved in a formatted file. If 2, an unformatted file is created.	unitless
SUMQ	RUNKUT	Net flow into or out of a junction.	ft^3/sec
*SURF(J)	DYNHYD RUNKUT	Surface area of junction J.	ft^2
SXX(F,J)	REGAN	Sum of X squared in normalized regression analysis equations.	unitless
SXY(J)	REGAN	Sum of X times Y in normalized regression analysis equations.	ft

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
T	DYNHYD	Total elapsed time. Initialized to equal TZERO and is incremented by DELT at the start of each time step.	sec
T2	DYNHYD RUNKUT	Total elapsed time for one half step computation.	sec
TEND	DYNHYD SEAWRD	Ending time of simulation.	hr
TIME	DYNHYD	Total time.	sec
TNEXTC	RUNKUT	Counter. Determines if tidal cycle should start over.	sec
TREP(J)	SEAWRD	Number of times the tidal cycle has been repeated.	rep
TREPW	WIND	Number of times wind data has been repeated.	rep
TRSTRT	DYNHYD RESTRT	Total elapsed time.	sec
*TSHIFT	SEAWRD REGAN	Variable that allows the time scale for the inputs to be shifted (usually = 0).	hr
*TSTART(J)	SEAWRD RUNKUT	Starting time for tidal input.	hr
TVEL (N,NA)	SUMRY1	Average velocity in channel N. (=AVGVEL).	ft/sec
TZERO	DYNHYD SEAWRD WIND	Time at which computations begin. Allows starting point to be anywhere on tidal cycle.	hr
VEL(N,1)	SUMRY1,2	Velocity at channel N.	ft/sec
*VFLOW (I,K)	DYNHYD SUMRY2	Flow value at increment K in variable flow record I. Negative values indicate inflow. Linear interpolation is used to derive flow values between increment K and K + 1.	ft^3/sec

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
*V(N)	DYNHYD WIND RUNKUT SUMRY1,2	Mean velocity in channel N.	ft/sec
VOL(J)	DYNHYD RUNKUT SUMRY1,2	Volume of junction J (average depth * surface area).	ft^3
VQ(I,J)	DYNHYD	Incremental flow in junction.	ft^3/ sec
VQIN(J)	DYNHYD RUNKUT	Sum of variable flows into each junction.	ft^3/ sec
VT(N)	RUNKUT	2/PERIOD.	hr^{-1}
WANGL	WIND	Wind direction relative to channel direction.	radians
WDELTA	WIND	Angle change between two consecutive wind data points.	radians
WDELTS	WIND	Wind speed change between two consecutive data points.	ft/sec
WDELTT	WIND	Time change between two consecutive data points.	sec
*WDIR(I)	WIND	Wind direction (degrees from North).	degrees
WINDA	WIND	Local interpolated wind angle.	degrees
WINDL	WIND	Local interpolated wind speed.	ft/sec
*WINDS(I)	WIND	Wind speed.	ft/sec
WRSQ	WIND	Relative wind speed (squared).	ft^2/ sec
W(SP)	SEAWRD	Frequency (2 * TLY/tidal period).	hr^{-1}
WSLOPA	WIND	Slope of line connecting two consecutive wind angle data points.	unit-less
WSLOPS	WIND	Slope of line connecting two consecutive wind speed data points.	unit-less

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
WTIM(I)	WIND	Time corresponding to WINDS(I) and WDIR(I).	sec
X(J)	REGAN	Coefficients for tidal cycle equation.	unit-less
*Y(J)	REGAN MEAN	Initial head for junction J in reference to a datum.	ft
*YSCALE	SEAWRD REGAN	Scale factor; defaults to 1.	unit-less
YSUM	MEAN	Summation of transformed head.	ft
YT(J)	DYNHYD RUNKUT	Head at junction J during one-half time step.	ft
YTMPS	DYNHYD	Sum of all heads for each junction.	ft
*ZDAY	DYNHYD	Beginning day of simulation.	day
*ZHR	DYNHYD	Beginning hour of simulation.	hr
*ZMIN	DYNHYD	Beginning minute of simulation.	min

2.3. THE BASIC WATER QUALITY MODEL

2.3.1 Introduction

This section describes the input required to run the WASP water-quality program. To arrange the input into a logical format, the data are divided into 16 groups, A through P.

A - Model Identification and System Bypass
B - Exchange Coefficients
C - Volumes
D - Flows
E - Boundary Concentrations
F - Waste Loads
G - Environmental Parameters
H - Chemical Constants
I - Time Functions
J - Initial Concentrations
K - Stability and Accuracy Criteria
L - Intermediate Print Control

M - Integration Control
N - Print Tables
O - Time Plots
P - Spatial Plots

The following is a brief explanation of each data group:

DATA GROUP A is generally for model identification and contains system bypass options. The user must specify the number of segments and the number of systems (EUTRWASP-8 systems, TOXIWASP-2 systems), refer to Table 19 for listings. Also, Data Group A contains information concerning location of initial concentration and volume data.

TABLE 19. EUTROWASP SYSTEMS

1. AMMONIA NITROGEN
2. NITRATE NITROGEN
3. ORTHO-PHOSPHATE PHOSPHORUS
4. PHYTOPLANKTON CARBON
5. CARBONACEOUS BOD
6. DISSOLVED OXYGEN
7. ORGANIC NITROGEN
8. ORGANIC PHOSPHORUS

TOXIWASP SYSTEMS

1. CHEMICAL
2. SEDIMENT

DATA GROUP B contains dispersive exchange coefficient information. Dispersion occurs between segments and along a characteristic length.

DATA GROUP C supplies initial segment volume information.

DATA GROUP D supplies flow information between segments. Flows may be constant or variable.

DATA GROUP E is a listing of concentrations for each system at the boundaries. All system concentrations must be supplied for each boundary.

DATA GROUP F defines the waste loads and segments that receive the waste loads. Loads may represent point or diffuse sources, and may be constant or variable.

DATA GROUP G contains appropriate environmental characteristics of the water body. TOXIWASP requires 18 parameters per segment, and EUTRWASP requires 13. These parameters are spatially variable.

DATA GROUP H contains appropriate chemical characteristics or constants. TOXIWASP requires 66 constants, and EUTRWASP requires 48 constants.

DATA GROUP I contains appropriate environmental or kinetic time functions. TOXIWASP requires 5 time functions, and EUTRWASP requires 14.

DATA GROUP J is a listing of initial concentrations for each segment and each system.

DATA GROUP K contains maximum and minimum concentrations for each system. If the system concentration exceeds this specification, the model will shut down and notify the user.

DATA GROUP L allows the user to have tables printed during the simulation. The system, segment and time interval must be specified.

DATA GROUP M supplies the program with the time step and ending time. The program allows different time steps throughout simulation. User must specify number of time steps to be used, step size, and period of time this time step applies.

DATA GROUP N controls the tabular output. EUTRWASP has 4 display variables per system, and TOXIWASP has 8 display variables per system. Refer to Tables 20 and 21 for a listing. These display variables may be printed for any of the segments.

DATA GROUP O allows the user to plot any variable against time for any segment. The maximum number of time curves on any one plot is 5, and one may have as many plots as desired.

DATA GROUP P allows user to plot and overlay predicted and observed variable data for any specific time. The maximum number of curves on any one spatial plots is 5.

2.3.2 WASP3 Data Group Descriptions

2.3.2.1 DATA GROUP A: Model Identification and System Bypass Option--

VARIABLES

Record 1--Model Identification

MODEL = model designation.

ISER = series designation.

IRUN = run number.

NOSEG = number of model segments.

TABLE 20. EUTRWASP DISPLAY VARIABLES

SYSTEM 1

1. NH3: Ammonia, mg/L
2. FLOW: Flow, MCF/day
3. STP: Ambient segment temperature, °C
4. PNH3GI: Ammonia preference factor

SYSTEM 2

1. NO3: Nitrate plus nitrate nitrogen, mg/L
2. TN: Total nitrogen, mg/L
3. TIN: Total inorganic nitrogen, mg/L
4. XEMP1: Nitrogen limitation factor for phytoplankton growth

SYSTEM 3

1. OPO4: Total ortho-phosphate phosphorus, mg/L
2. TP: Total phosphorus, mg/L
3. LIMIT: Nutrient limitation indicator
   ("+" = nitrogen, "-" = phosphorus)
4. XEMP2: Phosphorus limitation factor for phytoplankton growth

SYSTEM 4

1. TCHLAX: Phytoplankton chlorophyll a, ug/L
2. PHYT: Phytoplankton carbon, mg/L
3. RLIGHT: Light limitation factor for phytoplankton growth
4. RNUTR: Nutrient limitation factor for phytoplankton growth

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TABLE 20. EUTRWASP DISPLAY VARIABLES (Continued)

SYSTEM 5

1. CBOD: Carbonaceous BOD, mg/L
2. UBOD: Ultimate (30 day) BOD, mg/L
3. SOD: Sediment oxygen demand, g/m^2.day
4. BOD5: Five day BOD, mg/L

SYSTEM 6

1. DO: Dissolved oxygen, mg/L
2. DODEF: Dissolved oxygen deficit, mg/L
3. DOMIN: Minimum diurnal DO value, mg/L
4. DOMAX: Maximum diurnal DO value, mg/L

SYSTEM 7

1. ON: Organic nitrogen, mg/L
2. TON: Total organic nitrogen, mg/L
3. KA: Reaeration rate constant, day^{-1}
4. GPP: Ambient phytoplankton growth rate, day^{-1}

SYSTEM 8

1. OP: Organic phosphorus, mg/L
2. TOP: Total organic phosphorus, mg/L
3. RATIO: Inorganic nitrogen to phosphorus ratio
4. SKE: Ambient light extinction coefficient, ft^{-1}

TABLE 21. TOXIWASP DISPLAY TABLES

SYSTEM 1

1. CHEM: Chemical concentration, mg/L
2. CHEM1: Chemical dissolved in water phase, mg/L
3. CHEMS: Chemical sorbed onto sediment, mg/L
4. CHEMB: Chemical sorbed onto biological phase, mg/L
5. ALPHA(1): Dissolved fraction
6. ALPHA(2): Sorbed (sediment) fraction
7. XMASS: Mass of chemical in segment, kg
8. BMASS: Mass of chemical lost from segment due to burial or volatilization, kg

SYSTEM 2

1. SED: Sediment concentration, mg/L
2. DEPTHG: Segment depth, ft
3. TOTKL: Total first-order decay rate constant, day^{-1}
4. PHOTKL: Photolysis decay rate constant, hr^{-1}
5. HYDRKL: Hydrolysis decay rate constant, hr^{-1}
6. BIOLKL: Biodegradation decay rate constant, hr^{-1}
7. OXIDKL: Oxidation decay rate constant, hr^{-1}
8. VOLKL: Volatilization decay rate constant, hr^{-1}

NOSYS = number of systems.

LISTG = 0, print input data for exchange coefficients, volumes, flows, and boundary conditions on the principal output device.

= 1, do not print input data for exchange coefficients, volumes, flows, and boundary conditions.

LISTC = 0, print input data for forcing functions, segment parameters, constants, miscellaneous time functions, and initial conditions on the principal output device.

= 1, do not print input for forcing functions, segment parameters, constants, miscellaneous time functions, and initial conditions.

ICRD = file number containing initial conditions. If equal to 5, concentrations are read from data set. If equal to 8, concentrations are read from a file created by Subroutine RESTART from a previous run.

DAY = beginning day of simulation (day).

HR = beginning hour of simulation (hour).

MIN = beginning minute of simulation (min).

TITLE = Name of data group.

MODEL, ISER, IRUN and TITLE assist the user in maintaining a log of computer simulations, but are not actually used by the WASP program.

Record 2--Title Information

TITLE = Description of the water body (to be printed on the output).

Record 3--Simulation Option

TITLE = Description of simulation (to be printed on the output).

Record 4--Systems Bypass Option

SYSBY(K) = 0, perform the kinetic and transport phenomena associated with system K (numerically integrate the differential equations).

= 1, bypass all kinetic and transport phenomena associated with system K (concentrations read as initial conditions

There will be NOSYS entries in Record 4 (K = 1, NOSYS).

ORGANIZATION OF RECORDS

Each record in Data Group A is input once; therefore, Data Group A will consist of the first four lines of data. Because Record 4 can contain 40 entries (I2 format), all NOSYS entries for SYSBY(K) will fit on one line.

2.3.2.2 DATA GROUP B: Exchange Coefficients

The exchange coefficients may be input in one of two basic ways. The first reads in bulk exchange rates directly whereas the second calculates them from input dispersion coefficients and accompanying cross-sectional areas and characteristic lengths. There are six data input options. Records 1 and 2, described below, are identical in all six data group options. The variable IROPT, in Record 1, determines which option to use. The remaining records are described under each data group.

VARIABLES

Record 1--Data Input Option

IROPT = 1, constant exchange rates.

= 2, all exchange rates proportional to one piecewise linear approximation.

= 3, each exchange rate represented by its own piecewise linear approximation.

= 4, constant exchange rates calculated from the dispersion coefficient, cross-sectional area, and characteristic lengths specified for each interface.

= 5, all exchange coefficients proportional to one piecewise linear approximation, calculated from a piecewise linear dispersion coefficient approximation, respective cross-sectional areas, and characteristic lengths.

= 6, each exchange rate proportional to its own piecewise linear approximation, calculated from a piecewise linear approximation for the dispersion coefficients, cross-sectional areas, and characteristic length specified for each interface.

NOR = number of exchange rates.

If no exchange rates are to be read, set NOR equal to zero, and continue with DATA Group C.

TITLE = Name of data group.

Record 2--Scale and Conversion Factors

SCALR = scale factor for exchange coefficients. All exchange coefficients will be multiplied by this factor.

CONVR = units conversion factor for exchange coefficients. Exchange coefficients are expected to be in million cubic feet per day in options 1, 2 and 3 (B.1, B.2 and B.3). If the exchange coefficients are given in SI units (cubic meters per second), this factor will be 3.051.

Options B.4, B.5 and B.6 require the dispersion coefficient to be in square miles per day, the area in square feet, and the length in feet. The conversion of sq. mi. - feet/day to MCF/day for options 4, 5, and 6 is handled internally in WASP. If the dispersion coefficient, area and length are given in square meters per day, square meters and meters, respectively, CONVR will be 1.267×10^{-6}.

2.3.2.2.1 DATA GROUP B.1

VARIABLES

Record 3--Exchange Coefficients

BR(K) = exchange coefficient between segments IR(K) and JR(K) in million cubic feet per day.

IR(K), JR(K) = segments between which exchange takes place. The order of the segments is not important; if a segment exchanges with a boundary, the boundary is specified as zero.

K = 1, NOR

Record 4--Exchange Bypass Option

RBY(K) = 0, exchange phenomena occurs in system K.

= 1, bypass exchange phenomena for system K (effectively set all exchange coefficients equal to zero for system K).

K = 1, NOSYS

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in Data Group B.1, occupying one line each. Record 3, however, is repeated as many times as needed to satisfy NOR sets of BR(K), IR(K) and JR(K). For example, if NOR = 4, Record 3 would occupy one line of data, since four entries fit on one 80-space line. NOR = 10 would require three lines of data. No matter how many physical lines are used to complete NOR entries, all the lines are considered "Record 3".

After NOR entries have been entered in Record 3, the following line begins Record 4. All NOSYS entries will fit on one line.

2.3.2.2.2 DATA GROUP B.2

VARIABLES

Record 3--Exchange Coefficient Data

BR(K) = ratio of the exchange coefficient between segments IR(K) and JR (K) to the piecewise linear approximation.

IR(K), JR(K) = segments between which exchange takes place. The order of the segments is not important; if a segment exchanges with a boundary, the boundary is specified as zero.

K = 1, NOR

Record 4--Number of Breaks

NOBRK = number of values and times used to describe the piecewise linear approximation to the time function.

Record 5--Piecewise Linear Approximation

RT(K) = value of the approximation at time T(K), in million cubic feet per day.

T(K) = time in days; if the length of the simulation exceeds T(NOBRK), the piecewise linear approximation will repeat itself, starting at time T(1); i.e., the approximation is assumed to be periodic with period equal to T(NOBRK), this holds true for all piecewise linear functions time.

K = 1, NOBRK

Record 6--Exchange Bypass Option

RBY(K) = 0, exchange phenomena occurs in system K.

= 1, bypass exchange phenomena for system K (effectively set all exchange coefficients equal to zero for system K).

K = 1, NOSYS

ORGANIZATION OF RECORDS

In Data Group B.2, Records 1 and 2 are entered once. Record 3, however, will be repeated until NOR sets of BR(K), IR(K) and JR(K) are satisfied. Four sets will fit on one 80-space line (see the format listed for Record 3 in the accompaning tables). All the physical lines containing the BR(K), IR(K) and JR(K) data are considered "Record 3", even though more than one "record" (line) may actually be used.

After NOR sets have been entered, input Record 4 on the next line. Record 5, starting on the line after Record 4, will continue as Record 3 did, repeating until NOBRK sets of RT(K) and T(K) are entered. Four sets will fit on one 80-space line, as indicated in the table.

When NOBRK sets have been entered, input record 6 on the following line. Record 6 will have NOSYS entries.

2.3.2.2.3 DATA GROUP B.3

VARIABLES

Record 3--Exchange Placement

IR(K), JR(K) = segments between which exchange takes place. The order of the segments is not important; if a segment exchanges with a boundary, the boundary is specified as zero.

NOBRK = number of values and times used to describe the piecewise linear approximation. All exchanges must have the same number of breaks, and all breaks must occur at the same time relative to each other.

K = 1, NOR

Record 4--Piecewise Linear Approximation

RT(K) = value of the piecewise linear approximation at time T(K) in million cubic feet per day.

T(K) = time in days. All break times must agree for all segments, i.e., T(1) must be the same for all exchanges, T(2) must be the same for all exchanges, etc.

K = 1, NOBRK

Record 5--Exchange Bypass Options

RBY(K) = 0, exchange phenomena occur in system K.

= 1, bypass exchange phenomena for system K (effectively set all exchange coefficients equal to zero for system K).

K = 1, NOSYS

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in Data Group B.3 in the format listed in Table B.3. Records 3 and 4, grouped together, are repeated until NOR pairs have been entered. Within each Record 3-Record 4 set, Record 3 is input once and Record 4 is repeated, as necessary, until NOBRK sets of RT(K) and T(K) have been entered. Four sets of RT(K) and T(K) will fit on each 80-space line.

After NOR sets of Records 3 (with accompanying Record 4's) have been input, enter record 5. Record 5 will occupy one line and have NOSYS entries.

2.3.2.2.3 DATA GROUP B.4

Record 3--Data to Calculate Exchange Coefficients

E(K) = dispersion coefficient for the interface between segment IR(K), and JR(K) in square, miles/day.

A(K) = the interfacial cross-sectional area between segments IR(K) and JR(K), in square feet.

IL(K) = the length of segment IR(K), with respect to the IL(K)-JL(K) interface, in feet.

JL(K) = the length of segment JR(K) in the relation to the IR(K)-JR(K) interface, in feet. If a segment exchanges with a boundary, the characteristic length of the boundary should be set equal to the length of the segment with which it is exchanging.

IR(K), JR(K) = segments between which exchange takes place. The order of the segments is not important; if a segment exchanges with a boundary, the boundary is specified as zero.

K = 1, NOR

Record 4--Exchange Bypass Option

RBY(K) = 0, exchange phenomena occurs in system K.

= 1, bypass exchange phenomena for system K (effectively set all exchange coefficients equal to zero for system K.

K = 1, NOSYS

ORGANIZATION OF RECORDS

As in all the B data groups, Records 1 and 2 are entered once in Data Group B.4. Record 3 is repeated as necessary until NOR sets of E(K), A(K), IL(K), JL(K), IR(K) and JR(K) have been entered (two sets per line). After NOR sets are input, enter record 4 on the following line. Record 4 has NOSYS entries.

2.3.2.2.5 DATA GROUP B.5

VARIABLES

Record 3--Data to Calculate Exchange Coefficients

E(K) = the ratio of the dispersion coefficient between segment IR(K) and JR(K) to the piecewise linear approximation.

A(K) = the interfacial cross-sectional area between segments IR(K) and JR(K), in square feet.

IL(K) = the length of segment IR(K) in relation to the IR(K)-JR(K), in square feet.

JL(K) = the length of segment JR(K) in relation to the IR(K)-JR(K) interface, in feet. If a segment exchanges with a boundary, the characteristic length of the boundary should be set equal to the length of the segment with which it is exchanging.

IR(K), JK(K) = segments between which exchange takes place. The order of the segments is not important.

K = 1, NOR

Record 4--Number of Breaks

NOBRK = number of values and times used to describe the piecewise linear approximation to the time function.

Record 5--Piecewise Linear Approximation

RT(K) = value of the piecewise linear approximation at time T(K), in square miles/day.

T(K) = time in days.

K = 1, NOBRK

Record 6--Exchange Bypass Option

RBY(K) = 0, exchange phenomena occurs in system K.

= 1, bypass exchange phenomena for system K (effectively sets all exchange coefficients equal to zero for system K).

K = 1, NOSYS

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in Data Group B.5. Record 3 uses as many lines as needed to input NOR sets of E(K), A(K), IL(K), JL(K), IR(K) and JR(K). Two sets will fit on each 80-space line. Record 4, following Record 3, occupies one line. Record 5 uses as many lines as needed to enter NOBRK sets of RT(K)and T(K). Four RT(K)-T(K) pairs can be entered on each line. After NOBRK sets have been entered, input record 6 on the following line. Record 6 has NOSYS entries.

2.3.2.2.6 DATA GROUP B.6

VARIABLES

Record 3--Exchange Data

IR(K), JR(K) = segments between which exchange takes place. The order of the segments is not important.

NOBRK = number of values and times used to describe the piecewise linear approximation. All NOR exchanges must have the same number of breaks, and all breaks must occur at the same time relative to one another.

K = 1, NOR

Record 4--Piecewise Linear Approximation

RT(K) = value of the piecewise linear approximation at time T(K), in square miles/day.

T(K) = time in days; all break times must agree for all segments, i.e., T(1) must be the same for all exchanges, T(2) must be the same for all exchanges, etc.

K = 1, NOBRK

Record 5--Cross-Sectional Area, Characteristic Lengths

A(K) = the interfacial cross-sectional area between segment IR(K) and JR(K) in square feet.

IL(K) = the length of segment IR(K) in relation to the IR(K)-JR(K) interface, in feet.

JL(K) = the length of segment JR(K) in relation to the IR(K)-JR(K) interface in feet.

K = 1, NOR

If a segment exchanges with a boundary, the characteristic length of the boundary should be set equal to the length of the segment with which it is exchanging.

Record 6--Exchange Bypass Option

RBY(K) = 0, exchange occurs in system K.

= 1, bypass exchange phenomena for system K (effectively set for all exchange coefficients equal to zero for system K).

ORGANIATION OF RECORDS

Records 1 and 2 are entered once in Data Group B.6. Records 3, 4 and 5 are a set and are repeated NOR times. Within each set, Record 3 will be entered once (i.e., occupy one line) and record 5 will be entered once. Record 4, having NOBRK entries, will use multiple lines. Four entries will fit on each 80-space line. Records 3, 4 and 5 are input sequentially in each NOR set.

After NOR sets of Records 3, 4 and 5 have been entered, input Record 6 on the following line. Record 6 has NOSYS entries.

2.3.2.3 DATA GROUP C: Volumes

VARIABLES

Record 1--Preliminary Data

IVOPT = 1, constant volumes.

= 2, 3 volumes adjusted to maintain flow continuity.

TITLE = Name of data group.

Record 2--Scale Factor for Volumes

SCALV = scale factor for volumes. All volumes will be multiplied by this factor.

CONVV = scale factor for volumes. Volumes are expected in million cubic feet (MCF). If volumes are given in SI units (cubic meters), this factor will be 3.531 x 10^{-5}.

Record 3--Volumes of Segments

VOL(K) = volumes of segment K, in million cubic feet.

K = 1, NOSEG (from Card Group A)

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in Data Group C. Record 3 is repeated, as needed, until NOSEG entries are input. Eight entries will fit on one 80-space line. If ICRD = 8 in Data Group A, then volumes are read from the restart file (RESTART.OUT), and Record 3 should not be included in the input data set.

2.3.2.4 DATA GROUP D: Flows

Data Group D consists of the flows that are used in the model. There are four options available (D.1, D.2, D.3, and D.5). Records 1 and 2, discussed first, are the same in all four options. IQOPT, in Record 1, determines which option to use. The remaining records are explained under each data group.

VARIABLES

Record 1--Data Input Option; Number of Flows

IQOPT = 1, constant flows.

= 2, all flows proportional to one piecewise linear approximation.

= 3, each flow is represented by its own piecewise linear approximation.

= 4, flows are read in from an unformatted file (SUMRY2.OUT) created by DYNHYD3.

= 5, flows are read in from an unformatted file created by DYNHYD3 (SUMRY2.OUT).

NOQ = number of flows.

TITLE = name of data group.

If no flows are to be input, set NOQ to zero, and go to Card Group E.

Record 2 -- Scale Factor for Flows

SCALQ = scale factor for flows. All flows will be multiplied by this factor.

CONVQ = units conversion factor for flows. Flows are expected to be in cubic feet per second (cfs). If flows are given in SI units (cubic meters per second), this factor will be 35.31.

2.3.2.3.1 DATA GROUP D.1

VARIABLES

Record 3--Flow Routing

BQ(K) = flow between segment IQ(K) and JQ(K) in cfs. WASP convention is: if the flow value is positive, then flow is from segment JQ(K) to IQ(K).

IQ(K) = upstream segment.

JQ(K) = downstream segment.

K = 1, NOQ

If flow is from a segment to a boundary, then JQ(K) is set equal to zero; if a flow is from a boundary to a segment, then IQ(K) is set equal to zero.

Record 4--Flow Bypass Option

QBY(K) = 0, flow tranport occurs in system K.

= 1, bypass the flow transport for system K (effectively set all flows equal to zero in system K).

K = 1, NOSYS

The flow bypass option permits the flow transport to be set equal to zero in one or more systems, while maintaining the flow regime in the remaining systems.

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in D.1, occupying one 80-space line each. Record 3 uses as many lines are needed to enter NOQ sets of BQ(K), IQ(K) and JQ(K). Four sets will fit on each line. Record 4 has NOSYS entries and occupies one line.

2.3.2.4.2 DATA GROUP D.2

VARIABLES

Record 3--Flow Routing

BQ(K) = ratio of the flow between segments IQ(K) and JQ(K) to the piecewise linear flow approximation.

IQ(K) = upstream segment.

JQ(K) = downstream segment.

K = 1, NOQ

If flow is from a segment to a boundary, then JQ(K) is set equal to zero; if a flow is from a boundary to a segment, then IQ(K) is set equal to zero.

Record 4--Number of Breaks

NOBRK = number of values and times used to describe the piecewise linear approximation.

Record 5--Piecewise Linear Flow

QT(K) = value of the piecewise linear approximation at time T(K), in cubic feet per second.

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the broken line function will repeat itself, starting at time T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK).

K = 1, NOBRK

Record 6--Flow Bypass Option

QBY(K) = 0, flow tranport occurs in system K.

= 1, bypass the flow transport for system K (effectively sets all flows equal to zero in system K).

K = 1, NOSYS

The flow bypass option permits the flow transport to be set equal to zero in one or more systems, while maintaining the flow regime in the remaining systems.

ORGANIZATION OF RECORDS

Record 1 and 2 are input once in D.2. Record 3 uses as many 80-space lines as needed to enter NOQ sets of BQ(K), IQ(K) and JQ(K). Four sets will fit on one line. After NOQ sets have been input, enter Record 4 on the following line. Record 5 will have NOBRK sets of QT(K)-T(K) and uses as many lines as necessary to enter them (four sets per line). Record 6 occupies one line and will have NOSYS entries.

2.3.2.4.3 DATA GROUP D.3

VARIABLES

Record 3--Flow Routing

IQ(K) = upstream segment flow from segment IQ(K) to JQ(K), assuming positive flow.

JQ(K) = downstream segment flow from segment JQ(K), assuming positive flow.

NOBRK = number of values and times used to describe the broken line approximation. All NOQ flows must have the same number of breaks, and all breaks must occur at the same time relative to one another.

K = 1, NOQ

Record 4--Piecewise Linear Approximation

QT(K) = value of the piecewise linear flow approximation at time T(K) in cfs.

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the broken line function will repeat itself, stating at time, T(1). All break times must agree for all flows, i.e., T(1) must be the same for all flows, T(2) must be the same, etc.

K = 1, NOBRK

Record 5--Flow Bypass Option

QBY(K) = 0, flow transport occurs in system K.

= 1, bypass the flow transport for system K (effectively sets all flows equal to zero in system K).

K = 1, NOSYS

The flow bypass option permits the flow transport to be set equal to zero in one or more systems, while maintaining the flow regime in the remaining systems.

ORGANIZATION OF RECORDS

As in the other D data groups, Records 1 and 2 are entered once in Data Group D.3, using one 80-space line for each record. Records 3 and 4 are then grouped together and repeated NOQ times. Within each set, Record 3 is input once (using one line) and Record 4 uses as many lines as needed to enter NOBRK sets of QT(K)-T(K). Four QT(K)-T(K) sets will fit on one line.

After NOQ sets of Record 3 - Record 4 have been input, enter Record 5 on the following line. Record 5 will have NOSYS entries.

2.3.2.4.4 DATA GROUP D.5

VARIABLES

Record 3--Seaward Boundaries

NSEA = number of downstream (seaward) boundary segments (same as in hydrodynamic simulation).

JSEA(I) = segment numbers for downstream boundary segments.

I = 1, NSEA

Record 4--Junction-Segment Map

JUNSEG(I) = segment number corresponding to hydrodynamic junction I.

I = 1, NJ

Record 5--Flow Bypass Option

QBY(K) = 0, flow transport occurs in system K.

= 1, bypass the flow transport for system K (effectively set all flows equal to zero in system K).

ORGANIZATION OF RECORDS

As in other D data groups, Records 1 and 2 are entered once in Data Group D.5, using one 80-space line for each record. Records 3, 4, 5 and 6 follow in order. Record 4 will be repeated enough times to handle NJ entries. Record 5 will have NOSYS entries.

2.3.2.5 DATA GROUP E: Boundary Concentrations

Data Group E is repeated, in its entirety, NOSYS times. There are three options for Data Group E (E.1, E.2 and E.3). Each time E is repeated, a different option may be used.

Records 1 and 2 are identical in all three options. IBCOP(K), in Record 1, determines the option for each system.

VARIABLES

Record 1--Data Input Option--Number of Boundary Conditions

IBCOP(K) = 1, constant boundary conditions.

= 2, all boundary conditions proportional to one piecewise linear approximation.

= 3, each boundary condition represented by its own piecewise linear approximation.

NOBC(K) = number of boundary conditions used for system K.

TITLE = name of data group

K = 1, NOSYS

If no boundary conditions are to be input, set NOBC(K) equal to zero and either continue with the next system or go to the next card group.

Record 2--Scale Factor for Boundary Conditions

SCALB = scale factor for boundary conditions. All boundary conditions will be multiplied by this factor.

CONVB = unit conversion factor for boundary conditions. Boundary conditions are expected to be in milligrams per liter (mg/l). If boundary conditions are given in SI units (grams ber cubic meter), CONVB will be 1.0.

2.3.2.5.1 DATA GROUP E.1

VARIABLES

Record 3--Boundary Conditions

BBC(K) = boundary condition of segment IBC(K) in mg/l.

IBC(K) = segment number to which boundary condition BBC(K) is to be applied.

K = 1, NOBC

ORGANIZATION OF RECORDS

Records 1 and 2 are input once in E.1. Record 3 has NOBC entries and is repeated as necessary until all are entered (five entries per 80-space line).

2.3.2.5.2 DATA GROUP E.2

VARIABLES

Record 3--Boundary Conditions

BBC(K) = ratio of the boundary condition for segment IBC(K) to the piecewise linear approximation.

IBC(K) = segment number.

K = 1, NOBC

Record 4--Number of Breaks

NOBRK = number of values and times used to describe the piecewise linear approximation.

Record 5--Piecewise Linear Boundary Conditions (Approx)

BCT(K) = value of the broken line approximation at time T(K) in mg/l.

T(K) = time at breaks in broken line approximation, in days.

K = 1, NOBRK

If the length of the simulation exceeds T(NOBRK), the piecewise linear approximation is repeated, starting at T(1), i.e., the approximation is assumed to be period equal to T(NOBRK).

ORGANIZATION OF RECORDS

In E.2, Records 1 and 2 are entered once. Record 3, having NOBC entries, uses as many 80-space lines as needed to input all entries. Five entries (one entry is one BBC(K)-IBC(K) set) will fit on one line. Record 4 uses one line. Record 5 has NOBRK entries and is repeated as necessary until all are entered. Four pairs of BCT(K)-T(K) will fit on each line.

2.3.2.5.3 DATA GROUP E.3

VARIABLES

Record 3--Boundary Conditions

IBC(K) = boundary segment number.

NOBRK(K) = number of values and times used to describe the broken line approximation. The number of breaks must be equal for all boundary conditions within a system.

K = 1, NOBC

Record 4--Piecewise Linear Bound. Cond. (Approx.)

BCT(K) = value of the boundary approximation at time T(K) in mg/l.

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the broken line approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic, with period equation to T(NOBRK). All break times must agree for all segment, i.e., T(1) must be the same for all exchanges, T(2) must be the same for all exchanges, etc.

K = 1, NOBRK

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in E.3. Records 3 and 4 are a set and are repeated NOBC times. Within each NOBC set, Record 3 is entered once and Record 4 is repeated until NOBRK entries are input. Four entries (four BCT(K)-T(K) pairs) will fit on each 80-space line.

2.3.2.6 DATA GROUP F: Waste Loads

Data Group F contains the loads used in the model. Like Data Group E, Data Group F is repeated NOSYS times for point source loads. F.1, F.2 or F.3 may be used each time F is repeated. Records 1 and 2 are identical in all three data groups; IWKOP(K) in Record 1 determines the data group used. Following complete specification of point source loads, nonpoint source loads will be read from Data Group F.4 if LOPT was set greater than zero.

VARIABLES

Record 1--Data Input Option; No. of Forcing Functions

IWKOP(ISYS) = 1, constant forcing functions.

= 2, all forcing functions are proportional to one piecewise linear approximation.

= 3, each forcing function represented by its own piecewise linear approximation.

NOWK(ISYS) = number of forcing functions used for system ISYS. Forcing functions may also be considered as sources (loads) or sinks of a water quality constituent. If no forcing functions are to be input, set NOWK(ISYS) to zero, and continue with next system or go to next data group.

LOPT = option to read in Data Group F.4 for nonpoint source loads. If LOPT is greater than zero, then Data Group F.4 will be read following completion of F.1, F.2, or F.3 for all systems. LOPT is entered for ISYS=1 only.

TITLE = name of data group.

Record 2--Scale Factor for Forcing Functions

SCALW = scale factor for forcing functions. All forcing functions will be multiplied by this factor.

CONVW = unit conversion factor for forcing functions. Forcing functions are expected to be in pounds per day. If forcing functions are given in SI units (kilograms per day), this factor will be 2.205.

2.3.2.6.1 DATA GROUP F.1

VARIABLES

Record 3--Forcing Functions

BWK(K) = forcing function of segment IWK(K), in pounds/day.

IWK(K) = segment number to which forcing function BWK(K) is to be applied.

K = 1, NOWK

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in F.1. Record 3 has NOWK entries and uses as many 80-space lines as needed to enter all NOWK entries. Five entries (five BWK(K)-IWK(K) pairs) will fit on one line.

2.3.2.6.2 DATA GROUP F.2

VARIABLES

Record 3--Forcing Functions

BWK(K) = ratio of the forcing function for segment IWK(K) to the piecewise linear approximation.

IWK(K) = segment number to which forcing function BWK(K) is to be applied.

K = 1, NOWK

Record 4--Number of Breaks

NOBRK = number of values and times used to describe the piecewise linear approximation.

Record 5--Piecewise Linear Approximation

WKT(K) = value of the forcing function at time T(K), in pounds/day.

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the forcing function approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK).

K = 1, NOBRK

ORGANIZATION OF RECORDS

In F.2, Records 1, 2 and 4 are entered once. Record 3 (entered before Record 4) has NOWK entries and will be repeated until all are input. Five entries (BWK(K)-IWK(K) pairs) will fit on one 80-space line. Record 5 has NOBRK entries and will be repeated until all are entered. Four entries (WKT(K)-T(K) pairs) will fit on each 80-space line.

2.3.2.6.3 DATA GROUP F.3

VARIABLES

Record 3--Forcing Functions

IWK(K) = segment number that has forcing function BWK(K).

NOBRK(K) = number of breaks used to describe the forcing function approximation. The number of breaks must be equal for all forcing functions within a system.

K = 1, NOWK

Record 4--Piecewise Linear Approximation

WKT(K) = value of the forcing function at time T(K), in pounds/day.

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic with period equal to T(NOBRK). All break times must agree for all segments; i.e., T(1) must be the same for all boundary conditions, T(2) must be the same for all boun. cond., etc.

K = 1, NOBRK

ORGANIZATION OF RECORDS

In F.3, Records 1 and 2 are input once. Records 3 and 4 are a set and are repeated (as a set) NOWK times. Within each set, Record 3 is entered once and Record 4 is repeated until all NOBRK entries are entered. Four entries (WKT(K)-T(K) pairs) will fit on each 80-space line.

2.3.2.6.4 DATA GROUP F.4

VARIABLES

Record 1--Number of Runoff Loads, Initial Day

NOWKS = number of segments receiving runoff loads.

NPSDAY = the time in the runoff file corresponding to the initial simulation time, in days.

Record 2--Scale Factor for Runoff Loads

SCALN = scale factor for runoff loads. All runoff loads will be multiplied by this factor.

CONVN = unit conversion factor for runoff loads. Runoff loads are expected in pounds per day. If runoff loads are given in SI units (kilograms per day), this factor will be 2.205.

Record 3--Runoff Segments

INPS(J) = segment number to which runoff load J is applied.

J = 1,NOWKS

Record 4--Print Specifications

KT1 = initial day for which nonzero runoff loads from file NPS.DAT will be printed.

KT2 = final day for which nonzero runoff loads from file NPS.DAT will be printed.

KPRT(I) = indicator specifying whether nonzero runoff loads will be printed for each system. If KPRT(I) is greater than zero, then runoff loads will be printed for system I.

I = 1,NOSYS

ORGANIZATION OF RECORDS

Records 1 and 2 are entered once in Data Group F.4. Record 3 has NOWKS entries and uses as many 80-space lines as needed to enter all NOWKS segment numbers. Sixteen entries will fit on one line. Record 4 is entered once.

2.3.2.7 DATA GROUP G: Parameters

The definition of the parameters will vary, depending upon the structure and kinetics of the systems comprising each model. The input format, however, is constant.

VARIABLES

Record 1--Number of Parameters

NOPAM = number of parameters required by the model. If no parameters are to be input, set NOPAM to zero and go to Data Group H.

TITLE = name of data group.

Record 2--Scale Factors for Parameters

SCALP(K) = scale factor for parameter K.

K = 1, NOPAM

Record 3--Segment Parameters.

ANAME(K) = an optional one to five alphanumeric character descriptive name for parameter PARAM(ISEG,K).

PARAM(ISEG,K) = the value of parameter ANAME(K) in segment ISEG.

K = 1, NOPAM

ISEG = 1, NOSEG

ORGANIZATION OF RECORDS

Record 1 is input once in Data Group G, occupying one line. Record 2 has NOPAM entries. Eight entries will fit on one line; thus, Record 2 uses as many 80-space lines as needed to enter all NOPAM entries. Record 3 also has NOPAM entries and uses multiple lines. Five entries will fit per line.

2.3.2.8 DATA GROUP H: Constants--

The definition of the constants will vary, depending upon the structure and kinetics of the systems comprising each model.

VARIABLES

Record 1--Number of Constants

NCONS = number of constants required by the model.

TITLE = name of data group.

If no constants are to be input, set NCONS equal to zero and continue with the Data Group I.

Record 2--Constants

ANAME(K) = an optional one to five alpha-numeric character descriptive name for constant CONST(K).

CONST(K) = the value of constant ANAME(K).

K = 1, NCONS

ORGANIZATION OF RECORDS

Record 1 is entered once in Cata Group H. Record 2 has NCONS entries and uses as many 80-space lines as needed to input all NCONS entries. Five entries (ANAME(K)-CONST(K) pairs) will fit per line.

2.3.2.9 DATA GROUP I: Miscellaneous Time Functions--

The definition of the miscellaneous time function will vary depending upon the structure and the kinetics of the systems comprising each model. The input format, however, is constant.

VARIABLES

Record 1--Number of Time Functions

NFUNC = number of time functions required by the model. If no time functions are to be input, set NFUNC equal to zero and go to Card Group K.

TITLE = name of data group.

Record 2--Time Function Descriptions

ANAME(K) = an optional one to five alphanumeric character descriptive name for the time function K.

NOBRK(K) = number of breaks used to describe the time function K.

K = 1, NFUNC

Record 3--Time Functions

VALT(K) = value of the function at time T(K).

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK).

K = 1, NOBRK

ORGANIZATION OF RECORDS

Record 1 in entered once in Data Group I. Records 2 and 3, as a set, are repeated NFUNC times. Within each NFUNC set, Record 2 is input once and

Record 3 uses as many 80-space lines as needed to input NOBRK entries. Four entries (four VALK(K)-T(K) pairs) will fit on each 80-space line.

2.3.2.10 DATA GROUP J: Initial Concentrations--

The initial conditions are the segment concentration for the state variables at time zero (or the start of the simulation).

VARIABLES

Record 1--Title

TITLE = name of data group

Record 2--Initial Conditions

ANAME(K) = an optional one to five alpha-numeric character descriptive name for the initial condition in segment K of system ISYS.

C(ISYS,K) = initial concentration in segment K of system ISYS in the appropriate units (normally mg/l or ppm).

K = 1, NOSEG
ISYS = 1, NOSYS

ORGANIZATION OF RECORDS

Record 1 is input once in Data Group J. Record 2 is a set and will be repeated NOSYS times. Within each NOSYS set, there are NOSEG entries. Each NOSYS set will use as many 80-space lines as needed to input NOSEG entries. Five entries (ANAME(K)-C(ISYS,K) pairs) will fit one line. After NOSEG entries have been entered in a NOSYS set, begin the next NOSYS set on the following line.

Each NOSYS system must have initial conditions, even if the system is bypassed or the initial conditions are zero. If ICRD = 8 in Data Group A, then initial conditions are read from the restart file (RESTART.OUT), and Record 2 should not be included in the input data set.

2.3.2.11 DATA GROUP K: Stability and Accuracy Criteria--

VARIABLES

Record 1--Stability Criteria

CMAX(K) = stability criteria for system K, i.e., the maximum concentration (normal units mg/l or ppm) for system K which if exceeded by any segments in system K indicates that the numerical integration procedure has become unstable. If instability occurs, an appropriate message is printed and the integration procedure is terminated and a call is made to the display subroutines.

K = 1, NOSYS

Record 2--Accuracy Criteria

CMIN(K) = 0.0 for each system.

K = 1, NOSYS

ORGANIZATION OF RECORDS

In Data Group K, Records 1 and 2 each have NOSYS entries. Each record will use as many 80-space lines as needed to enter all NOSYS entries. Eight entries (CMAX(K) in Record 1; CMIN(K) in Record 2) will fit on one line.

2.3.2.12 DATA GROUP L: Intermediate Print Control--

There are two options for Data Group L (L.1 and L.2). Records 1 and 2 are identical in the two options. ISYS(1), in Record 3, determines the option. If ISYS(1) = 0, then option 2 is invoked. Otherwise, option 1 is used.

VARIABLES

Record 1--Number of Print Intervals

NPRINT = number of print intervals. NOTE: The maximum number of print outs = total prototype time/print interval + 1 (for time zero) must be equal to or less than the FORTRAN parameter MP that was used when compiling the program.

TITLE = name of data group.

Record 2--Print Intervals

PRINT(I) = print interval (day).

TPRINT(I) = final time for application of PRINT(I) (day).

I = 1,NPRINT

2.3.2.12.1 DATA GROUP L.1

VARIABLES

Record 3--Compartments (system - segment) to be Displayed

ISYS(K), ISEG(K) = system, segment combinations that the user wishes to have displayed during simulation - user may select a maximum of 8. All system-segment concentrations as well as other miscellaneous calculations may be displayed at the end of the simulation; see Card Group N.

K = 1, 8

ORGANIZATION OF RECORDS

In Data Group L.1, Record 1 is entered once. Record 2 contains four print interval-final time combinations per line. This record is repeated (NPRINT/4) + 1 times. Record 3 will have up to eight entries and use one 80-space line.

2.3.2.12.2 DATA GROUP L.2

VARIABLES

Record 3--Mass Check

IMCHK = 0 to invoke mass check option.

MSYS = system number for which a total mass balance analysis will be performed.

2.3.2.13 DATA GROUP M: Integration Control--

VARIABLES

Record 1--Integration Option - Negative Solution Option

INTYP = 1, user wishes the WASP program to determine the integration step size (based upon its own accuracy criteria). This option is not recommended.

= 2, the user will supply the integration step sizes that WASP will use. This option is recommended.

NEGSLN = 0, a user wishes to restrict integration to the positive plane only - this is the normal option selected.

= 1, user will permit the integration procedure to go negative - used for special applications (es., DO deficit, pH - alkalinity).

TITLE = name of data group.

Record 2--Time Warp Scale Factor - Starting Simulation Time

SCALT = time warp scale factor - not used.

TZERO = prototype time for start of simulation. This is usually equal to zero, but user may start at time other than zero (used to initialize any of the piecewise linear time functions). If DAY, HR, MIN are entered in Data Group A, this value is ignored.

Record 3--Number of Integration Step Sizes

NOSTEP = number of integration step sizes to be used in the simulation.

Record 4--Integration Step Size History

DT(K) = integration step size (normal units-days).

TIME(K) = time until which step size DT(K) will be used, then switching to DT(K+1) until TIME(K+1).

K = 1, NOSTEP

ORGANIZATION OF RECORDS

Records 1, 2 and 3 are input once in Data Group M, occupying one 80-space line each. Record 4 will use as many lines as needed to enter NOSTEP

2.3.2.14 DATA GROUP N: Print Tables--

This card group controls the output data.

VARIABLES

Record 1--Variable Names

ANAME(K) = a one to eight alpha-numeric character descriptive name for display variable K. The order of these names is determined via the assignment order in the user's kinetic subroutine.

TITLE = name of data group

K = 1,8

Record 2--Variable Number - Segment Numbers

VARNO = the position of the desired variables, to be displayed, in the WRITE file statement in the kinetic subroutine (see previous note).

SEG(K) = segment number to be displayed. Order of display is unimportant, i.e., need not be sequential.

K = 1, NOSEG

Record 3--Blank

Blank record.

ORGANIZATION OF RECORDS

Data Group N is repeated in its entirety NOSYS times. Within each NOSYS set, Record 1 is entered once. Record 2 may then be repeated as many times as the user wishes. Each record 2 entered will output a table of data for the variable designated in VARNO and the eight corresponding SEG(K)'s. The same variable may be used for VARNO again if the user wants to print data on eight more segments under that variable. The user may repeat this process for each of the eight variables listed in Record 1.

The variables in Record 2 do not have to be entered sequentially; for example, in the first "Record 2" entered, VARNO can equal 4 and the next "Record 2" can have VARNO = 2 or any other number one through eight. Thus, the user can arrange the output tables anyway he or she wishes.

The systems, however, must be input sequentially. After Record 1 and all the Record 2's the user wants displayed are input for NOSYS = 1, enter the blank line (Record 3) and then enter Record 1 for NOSYS = 2. Continue with the Record 2's for that system and the blank Record 3. Again, Record 2 in each NOSYS system can be repeated an infinite number of times and the blank record must be input between each subsequent NOSYS set.

2.3.2.15 DATA GROUP O: Printer Plot Display Cards (Time Plots)--

VARIABLES

Record 1--Number of Segments and Variables for Plot

NSPLT = number of segments to be plotted (maximum of five).

VARNO = the position of the desired variable to be plotted, in the WRITE file statement in the kinetic subroutine.

TITLE = name of data group.

Record 2--Plotting Scales

PMIN, PMAX = minimum and maximum values, respectively, to be used for this plot.

Record 3--Segment to be Plotted

SEG(K) = segment numbers to be plotted (a maximum of five segments per plot allowed)

Record 4--Blank

Blank record.

ORGANIZATION OF RECORDS

Data Group O will be entered once for each system 1 through NOSYS. Within each system, Records 1-3 are repeated for each plot the user wants to print from that system. Two plots are printed per page; therefore, Records 1-3 should be entered an even number of times within each NOSYS group. Each record will occupy one line.

After all sets of Records 1-3 have been input for NOSYS = 1, enter the blank Record 4 and then the data (Records 1-3) for NOSYS = 2. Continue in this manner until all systems have plotting data.

2.3.2.16 DATA GROUP P: Spatial Plots--

Card Group P controls plots from both predicted data and observed data.

VARIABLES

Record 1--Spatial Scale

RM1, RM2 = minimum and maximum river mile values, respectively, to be used for all spatial plots.

TITLE = name of data group.

Record 2--Segment River Miles to be Plotted

SEG(K) = segment number to be plotted.

RM(K) = river mile value for SEG(K).

K = 1, NOSEG

Record 3--Predicted Variable Plot Control Information

MXTIM = number of time selections to be included on this plot (maximum of 5).

IVAR = the position of the desired variable to be plotted in the WRITE file statement in the kinetic subroutine.

YSTR, YSTP = minimum and maximum values, respectively, to be used for the Y-axis of this plot.

SYSOPT = system number of the desired variable to be plotted.

OVRLAY = flag to cause this plot to be overlaid with the following plots:

= 0, causes this plot to be printed along (or with preceding plot, if OVRLAY on the preceding plot cards is set to 1).

= 1, causes this plot to be overlaid on the following plot. (Note: Although any number of plots can be overlaid, we suggest a maximum of three; YSTR and YSTP values should be compatible for overlaid plots.)

TITL1 = title for plot. When overlaying plots, the first two titles and the last title will be printed.

Record 4--Predicted Variable Plot Control Information

TIM(K) = time selections for this plot (1-MXTIM).

SYMTAB(K) = plot symbol associated with time TIM(K).

Record 5--Observed Data Plot Control Information

FLAG = flag to indicate observed data.

= 99999, plot the observed data.

IUNIT = unit device number where observed data are to be found (default = 5; optional unit numbers are 82-89).

YSTR, YSTP = minimum and maximum values, respectively, to use for the Y-axis of this plot.

NOOBS = number of observed data points for this plot.

OVRLAY = 0, causes this plot to be printed alone (or with preceeding plot, if OVRLAY on the preceding plot cards is 1).

= 1, causes this plot to be overlaid on the following plot.

TITL1 = title for this plot.

OBSSYM = plot symbol associated with observed data for this plot.

Record 6--River Mile - Observed Data Values

RIVMIL(K) = river mile location for observed data point "K".

VALUE(K) = observed value of variable at RIVMIL(K).

K = 1, NOOBS

Record 7--Format Specification for Data on "IUNIT"

FMT = format specification for observed river mile - observed data values on auxiliary input file IUNIT (specified on Record 5). Must begin and end with parentheses and contain valid formats, such as (2F5.0), (16F5.0) or (F5.0/F5.0).

ORGANIZATION OF RECORDS

Record 1 is entered once, occupying one line. Record 2 will use as many lines as needed to input NOSEG pairs of SEG(K)-RM(K); eight pairs may be entered per line. Records 3 and 4 are for plots from predicted data. Each will be entered once and occupy one line apiece. Any number of plots from predicted data can be printed by repeating Records 3 and 4.

To print plots from observed data, skip Records 3 and 4 and input Record 5. Record 5 is entered once and occupies one line. If IUNIT equals five or zero, use Record 6 and skip Record 7. Record 6 will use as many lines as necessary to enter NOOBS pairs of RIVMIL(K)-VALUE(K) (four pairs per line). If IUNIT equals 82-89, skip Record 6 and use Record 7. Record 7 will be entered once. Any number of plots from observed data can be printed by repeating Card Groups 5 and 6 or 5 and 7.

2.3.3 WASP3 Data Group Tables

DATA GROUP A

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	MODEL	I5	1-5	Model designation.
	ISER	I5	6-10	Series designation.
	IRUN	I5	11-15	Run number.
	NOSEG	I5	16-20	Number of segments.
	NOSYS	I5	21-25	Number of systems.
	LISTG	I5	26-30	Echo print suppression for B, C, D, E.
	LISTC	I5	31-35	Echo print suppression for F, G, H, I, J.
	ICRD	I5	36-40	File which contains flows.
	DAY	F5.0	41-45	Day to begin reading from file (day).
	HR	1X,F2.0	47-48	Hour to begin reading from file (hr).
	MIN	F2.0	49-50	Min to begin reading from file (min).
	TITLE	5A4	61-80	"A: Model options".
2	TITLE	20A4	1-80	Desc. of aquatic system.
3	TITLE	20A4	1-80	Desc. of simulation.
4	SYSBY(1)	I2	1-2	System bypass options.
	SYSBY(2)	I2	3-4	K = NOSYS
	.	.	.	
	.	.	.	
	.	.	.	
	SYSBY(K)	I2		

ORGANIZATION OF RECORDS:

$\boxed{1}$ $\boxed{2}$ $\boxed{3}$ $\boxed{4}$

DATA GROUP B.1

RECORD	VARIABLE	TYPE	COLUMN	SHORT DEFINITION
1	IROPT	I5	1-5	Exchange option = 1.
	NOR	I5	6-10	Number of exchange coefficients.
	TITLE	5A4	61-80	"B: Exchanges".
2	SCALR	F10.0	1-10	Scale factor for exchange coefficients
	CONVR	F10.0	11-20	Units conversion factor.
3	BR(K)	F10.0	1-10	Exchange coefficients.
	IR(K)	I5	11-15	Mixing segment K, K=1
	JR(K)	I5	16-20	Mixing segment K, K=1
	BR(K)	F10.0	21-30	K = 2
	IR(K)	I5	31-35	
	JR(K)	I5	36-40	
	BR(K)	F10.0	41-50	K = 3
	IR(K)	I5	51-55	
	JR(K)	I5	56-60	
	BR(K)	F10.0	61-70	K = 4
	IR(K)	I5	71-75	
	JR(K)	I5	76-80	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	BR(K)	F10.0	.	K = NOR
	IR(K)	I5	.	
	JR(K)	I5	.	
4	RBY(1)	I2	1-2	Exchange bypass option for each system.
	RBY(2)	I2	3-4	K = NOSYS
	.	.	.	
	.	.	.	
	.	.	.	
	RBY(NOSYS)	I2		

ORGANIZATION OF RECORDS:

|1| |2| |3|(NOR/4)|3| |4|

DATA GROUP B.2

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IROPT	I5	1-5	Exchange option = 2.
	NOR	I5	6-10	No. of exchange coefficients.
	TITLE	5A4	61-80	"B: Exchanges".
2	SCALR	F10.0	1-10	Scale factor for exch. coeff.
	CONVR	F10.0	11-20	Units conversion factor.
3	BR(K)	F10.0	1-10	Bulk exchange coefficients.
	IR(K)	I5	11-15	Mixing segment K.
	JR(K)	I5	16-20	Mixing segment K, K = 1
	BR(K)	F10.0	21-30	K = 2
	IR(K)	I5	31-35	
	JR(K)	I5	36-40	
	BR(K)	F10.0	41-50	K = 3
	IR(K)	I5	51-55	
	JR(K)	I5	56-60	
	BR(K)	F10.0	61-70	K = 4
	IR(K)	I5	71-75	
	JR(K)	I5	76-80	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	BR(K)	F10.0	.	K = NOR
	IR(K)	I5	.	
	JR(K)	I5	.	
4	NOBRK	I5	1-5	Number of values in the time function.
5	RT(K)	F10.0	1-10	Value of piecewise lin.
	T(K)	F10.0	11-20	approx. time in days; K = 1
	RT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	RT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	RT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	RT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	
6	RBY(1)	I2	1-2	Exchange bypass option for each system.
	RBY(2)	I2	3-4	
	.	.	.	
	.	.	.	
	.	.	.	
	RBY(NOSYS)	I2	.	

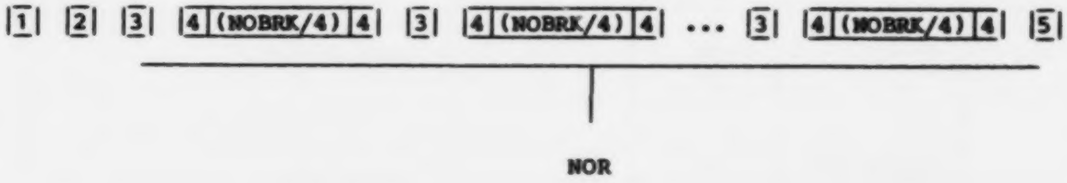
ORGANIZATION OF RECORDS:

$\boxed{1}\boxed{2}$ $\boxed{3}\boxed{(NOR/4)}\boxed{3}$ $\boxed{4}$ $\boxed{5}\boxed{(NOBRK/4)}\boxed{5}$ $\boxed{6}$

DATA GROUP B.3

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IROPT	I5	1-5	Exchange option = 3.
	NOR	I5	6-10	No. of exchange coefficients.
	TITLE	5A4	61-80	"B: Exchanges".
2	SCALR	F10.0	1-10	Scale factor for exch. coeff.
	CONVR	F10.0	11-20	Units conversion factor.
3	IR(I)	I5	1-5	Mixing segment K.
	JR(I)	I5	6-10	Mixing segment K.
	NOBRK(I)	I5	11-15	No. of values and times.
4	RT(K)	F10.0	1-10	value of piecewise lin.
	T(K)	F10.0	11-20	approx. time in days; K = 1
	RT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	RT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	RT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	RT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	
5	RBY(1)	I2	1-2	Exchange bypass option for each system.
	RBY(2)	I2	3-4	
	.	.	.	
	.	.	.	
	.	.	.	
	RBY(NOSYS)	I2		

ORGANIZATION OF RECORDS:



DATA GROUP B.4

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IROPT	I5	1-5	Exchange option = 4.
	NOR	I5	6-10	No. of exchange coefficients.
	TITLE	5A4	61-80	"B: Exchanges".
2	SCALR	F10.0	1-10	Scale factor for exch. coeff.
	CONVR	F10.0	11-20	Units conversion factor.
3	E(K)	F10.0	1-10	Dispersion factor; K = 1
	A(K)	F10.0	11-20	Cross sectional area.
	IL(K)	F5.0	21-25	Characteristic mixing length.
	JL(K)	F5.0	26-30	Characteristic mixing length.
	IR(K)	I5	31-35	Mixing segment K (upstream).
	JR(K)	I5	36-40	Mixing segment K (downstream).
	E(K)	F10.0	41-50	K = 2
	A(K)	F10.0	51-60	
	IL(K)	F5.0	61-65	
	JL(K)	F5.0	66-70	
	IR(K)	I5	71-75	
	JR(K)	I5	76-80	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	E(K)	F10.0	.	K = NOR
	A(K)	F10.0	.	
	IL(K)	F5.0	.	Continue until all exchange coefficients have been listed.
	JL(K)	F5.0		
	IR(K)	I5		
	JR(K)	I5		
4	RBY(1)	I2	1-2	Exchange bypass option for each system.
	RBY(2)	I2	3-4	
	.	.	.	
	.	.	.	
	RBY(NOSYS)	I2		

ORGANIZATION OF RECORDS:

$\boxed{1}$ $\boxed{2}$ $\boxed{3\,(NOR/2)\,3}$ $\boxed{4}$

DATA GROUP B.5

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IROPT	I5	1-5	Exchange option = 5.
	NOR	I5	6-10	No. of exchange coefficients.
	TITLE	5A4	61-80	"B: Exchanges".
2	SCALR	F10.0	1-10	Scale factor for each coeff.
	CONVR	F10.0	11-20	Units conversion factor.
3	E(K)	F10.0	1-10	Dispersion factor; K = 1
	A(K)	F10.0	11-20	Cross sectional area.
	IL(K)	F5.0	21-25	Characteristic mixing length.
	JL(K)	F5.0	26-30	Characteristic mixing length.
	IR(K)	I5	31-35	Mixing segment K (upstream).
	JR(K)	I5	36-40	Mixing segment K (downstream)
	E(K)	F10.0	41-50	K = 2
	A(K)	F10.0	51-60	
	IL(K)	F5.0	61-65	
	JL(K)	F5.0	66-70	
	IR(K)	I5	71-75	
	JR(K)	I5	76-80	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	E(K)	F10.0	.	K = NOR
	A(K)	F10.0	.	
	IL(K)	F5.0	.	
	JL(K)	F5.0		
	IR(K)	I5		
	JR(K)	I5		
4	NOBRK	I5	1-5	No. of values and times
5	RT(K)	F10.0	1-10	Value of piecewise lin.
	T(K)	F10.0	11-20	approx. time in days; K = 1
	RT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	RT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	RT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	RT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	
6	RBY(1)	I2	1-2	Exchange bypass option for
	RBY(2)	I2	3-4	each system.
	.	.	.	
	.	.	.	
	RBY(NOSYS)	I2		

ORGANIZATION OF RECORDS:

$\boxed{1}\boxed{2}$ $\boxed{3}\boxed{(NOR/2)}\boxed{3}$ $\boxed{4}$ $\boxed{5}\boxed{(NOBRK/4)}\boxed{5}$ $\boxed{6}$

DATA GROUP B.6

RECORD	VARIABLE	TYPE	COLUMN	SHORT DEFINITION
1	IROPT	I5	1-5	Exchange option = 6.
	NOR	I5	6-10	No. of exchange coefficients.
	TITLE	5A4	61-80	"B: Exchanges".
2	SCALR	F10.0	1-10	Scale factor for exch. coeff.
	CONVR	F10.0	11-20	Units conversion factor.
3	IR(K)	I5	1-5	Mixing segment K (upstream).
	JR(K)	I5	6-10	Mixing segment K (downsteam)
	NOBRK(K)	I5	11-15	No. of times in the time func
4	RT(K)	F10.0	1-10	Value of broken line approx; K = 1
	T(K)	F10.0	11-20	Time at breaks (in days)
	RT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	RT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	RT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	. .	. .	. .	. .
	RT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	
5	A(K)	F10.0	1-10	Cross sectional area.
	IL(K)	F10.0	11-20	Characteristic mixing length.
	JL(K)	F10.0	21-30	Characteristic mixing length.
6	RBY(1)	I2	1-2	Exchange bypass options for each system.
	RBY(2)	I2	3-4	
	. . .	. . .	. . .	
	RBY(NOSYS)	I2		

ORGANIZATION OF RECORDS:

|1|2| |3|4|(NOBRK/4)|4|5| |3|4|(NOBRK/4)|4|5|...|3|4|(NOBRK/4)|4|5| |6|

NOR

DATA GROUP C.1, C.2, C.3, C.4

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IVOPT	I5	1-5	Volume option number.
	NOV	I5	6-10	Number of volumes read.
	TITLE	5A4	61-80	"C: Volumes."
2	SCALV	E10.3	1-10	Scale Factor.
	CONVV	11-20	11-20	Units conversion factor.
3	VOL(K)	F10.0	1-10	Volume of segment (K); K = 1
	VOL(K)	F10.0	11-20	K = 2
	VOL(K)	F10.0	21-30	K = 3
	VOL(K)	F10.0	31-40	K = 4
	VOL(K)	F10.0	41-50	K = 5
	VOL(K)	F10.0	51-60	K = 6
	VOL(K)	F10.0	61-70	K = 7
	VOL(K)	F10.0	71-80	K = 8
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VOL(K)	F10.0		K = NOV

ORGANIZATION OF RECORDS:

|1|2| |3|(NOV/8)|3|

DATA GROUP C.4 (if NOV=0)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IVOPT	I5	1-5	Volume option number.
	NOV	I5	6-10	Number of volumes read = 0.
	TITLE	5A4	61-80	"C: Volumes."

ORGANIZATION OF RECORDS:

|1|

DATA GROUP D.1

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IQOPT	I5	1-5	Data input option number.
	NOQ	I5	6-10	Number of flows.
	TITLE	5A4	61-80	"D: Flows".
2	SCALQ	E10.3	1-10	Scale factor for flows.
	CONVQ	11-20	11-20	Units conversion factor.
3	BQ(K)	F10.0	1-10	Flows between segment IQ(K) and JQ(K); K = 1
	IQ(K)	I5	11-15	Upstream segment.
	JQ(K)	I5	16-20	downstream segment.
	BQ(K)	F10.0	21-30	K = 2
	IQ(K)	I5	31-35	
	JQ(K)	I5	36-40	
	BQ(K)	F10.0	41-50	K = 3
	IQ(K)	I5	51-55	
	JQ(K)	I5	56-60	
	BQ(K)	F10.0	61-70	K = 4
	IQ(K)	I5	71-75	
	JQ(K)	I5	76-80	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	BQ(K)	F10.0	.	K = NOV
	IQ(K)	I5	.	
	JQ(K)	I5	.	
4	QBY(K)	I2	1-2	Flow bypass option for system K; K = 1
	QBY(K)	I2	3-4	K = 2
	.	.	.	.
	.	.	.	.
	QBY(K)	I2	.	K = NOSYS

ORGANIZATION OF RECORDS:

|1| |2| |3|(NOQ/4)|3| |4|

DATA GROUP D.2

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IQOPT	I5	1-5	Data input option number.
	NOQ	I5	6-10	Number of flows.
	TITLE	5A4	61-80	"D: Flows".
2	SCALQ	E10.3	1-10	Scale factor for flows.
	CONVQ	E10.3	11-20	Units conversion factor.
3	BQ(K)	F10.0	1-10	Ratio of flow between seg. IQ(K) and JQ(K); K = 1
	IQ(K)	I5	11-15	Upstream segment.
	JQ(K)	I5	16-20	Downstream segment.
	BQ(K)	F10.0	21-30	K = 2
	IQ(K)	I5	31-35	
	JQ(K)	I5	36-40	
	BQ(K)	F10.0	41-50	K = 3
	IQ(K)	I5	51-55	
	JQ(K)	I5	65-60	
	BQ(K)	F10.0	61-70	K = 4
	IQ(K)	I5	71-75	
	JQ(K)	I5	76-80	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	BQ(K)	F10.0	.	K = NOV
	IQ(K)	I5	.	
	JQ(K)	I5	.	
4	NOBRK	I5	1-5	No. of values and times.
5	QT(K)	F10.0	1-10	Value of piecewise lin. appx.
	T(K)	F10.0	11-20	Time in days; K = 1
	QT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	QT(K)	F10.0	41-50	K = 3
	T(K(	F10.0	41-60	
	QT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	QT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	
6	QBY(K)	I2	1-2	Flow bypass option for system K; K = 1
	QBY(K)	I2	3-4	K = 2
	.	.	.	.
	.	.	.	.
	QBY(K)	I2	.	K = NOSYS

ORGANIZATION OF RECORDS:

|1|2| |3|(NOQ/4)|3| |4| |5|(NOBRK/4)|5| |6|

DATA GROUP D.3

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IQOPT	I5	1-5	Data input option number.
	NOQ	I5	6-10	Number of flows.
	TITLE	5A4	61-80	"D: Flows".
2	SCALQ	E10.3	1-10	Scale factor for flows.
	CONVQ	E10.3	11-20	Units conversion factor.
3	IQ(I)	I5	1-5	Upstream segment.
	JQ(I)	I5	6-10	Downstream segment.
	NOBRK(I)	I5	11-15	No. of values and times.
4	QT(K)	F10.0	1-10	Value of piecewise lin. appx.
	T(K)	F10.0	11-20	Time in days; K = 1
	QT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	QT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	QT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	QT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	
5	QBY(K)	I2	1-2	Flow bypass option for system K; K = 1
	QBY(K)	I2	3-4	K = 2
	.	.	.	.
	.	.	.	.
	QBY(K)	I2	.	K = NOSYS

ORGANIZATION OF RECORDS:

|1| |2| |3| |4|(NOBRK/4)|4| |3| |4|(NOBRK/4)|4|. . .|3| |4|(NOBRK/4)|4| |5|

NOQ

DATA GROUP D.4

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IQOPT	I5	1-5	Data input option number.
	NOQ	I5	6-10	Number of flows.
	TITLE	5A4	61-80	"D: Flows".
2	SCALQ	E10.3	1-10	Scale factor for flows.
	CONVQ	E10.3	11-20	Units conversion factor.
3	NSEA	I5	1-5	Number of downstream boundary segments.
	JSEA(I)	I5	6-10	Segment numbers for down-
	JSEA(I)	I5	11-15	stream boundaries.
	.	.	.	(1-NSEA)
	.	.	.	
	.	.	.	
4	JUNSEG(I)	I5	1-5	Segment number for hydro-
	JUNSEG(I)	I5	6-10	dynamic junction I.
	.	.	.	
	.	.	.	
	.	.	.	
5	QBY(K)	I2	1-2	Flow bypass option for system K; K = 1
	QBY(K)	I2	3-4	K = 2
	.	.	.	.
	.	.	.	.
	QBY(K)	I2	.	K = NOSYS

ORGANIZATION OF RECORDS:

|1| |2| |3| |4| |5|

DATA GROUP D.5

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IQOPT	I5	1-5	Data input option number.
	NOQ	I5	6-10	Number of flows.
	TITLE	5A4	61-80	"D: Flows".
2	SCALQ	E10.3	1-10	Scale factor for flows.
	CONVQ	E10.3	11-20	Units conversion factor.
3	NSEA	I5	1-5	Number of downstream boundary segments.
	JSEA(I)	I5	6-10	Segment numbers for downstream boundaries.
	JSEA(I)	I5	11-15	(1-NSEA)
	.	.	.	
	.	.	.	
	.	.	.	
4	JUNSEG(I)	I5	1-5	Segment number for hydrodynamic junction I.
	JUNSEG(I)	I5	6-10	
	.	.	.	
	.	.	.	
	.	.	.	
5	QBY(K)	I2	1-2	Flow bypass option for system K; K = 1
	QBY(K)	I2	3-4	K = 2
	.	.	.	.
	.	.	.	.
	QBY(K)	I2	.	K = NOSYS

ORGANIZATION OF RECORDS:

$\boxed{1}$ $\boxed{2}$ $\boxed{3}$ $\boxed{4}$ $\boxed{5}$

DATA GROUP E.1

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IBCOP(K)	I5	1-5	Data input options.
	NOBC(K)	I5	6-10	No. of boundary conditions.
	TITLE	5A4	61-80	"E: Boundary Concentrations".
2	SCALB	E10.3	1-10	Scale factor.
	CONVB	E10.3	11-20	Units conversion factor.
3	BBC(K)	F10.0	1-10	Boundary cond. of segment IBC(K); K = 1
	IBC(K)	I5	11-15	Segment number
	BBC(K)	F10.0	16-25	K = 2
	IBC(K)	I5	26-30	
	BBC(K)	F10.0	31-40	K = 3
	IBC(K)	I5	41-45	
	BBC(K)	F10.0	46-55	K = 4
	IBC(K)	I5	56-60	
	BBC(K)	F10.0	61-70	K = 5
	IBC(K)	I5	71-75	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	BBC(K)	F10.0	.	K = NOQ
	IBC(K)	I5	.	

ORGANIZATION OF RECORDS FOR E.1:

|1|2| |3|(NOBC(K)/5)|3|

Sequence of Records for "E" Card Groups:

|E1, E2, or E3| |E1, E2, or E3|...|E1, E2, or E3|

NOSYS

DATA GROUP E.2

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IBCOP(K)	I5	1-5	Data input options.
	NOBC(K)	I5	6-10	No. of boundary conditions.
	TITLE	5A4	61-80	"E: Boundaries".
2	SCALB	E10.3	1-10	Scale factor.
	CONVB	E10.3	11-20	Units conversion factor.
3	BBC(K)	F10.0	1-10	Ratio of bound. cond. for segment IBC(K); K = 1
	IBC(K)	I5	11-15	Segment number
	BBC(K)	F10.0	16-25	K = 2
	IBC(K)	I5	26-30	
	BBC(K)	F10.0	31-40	K = 3
	IBC(K)	I5	41-45	
	BBC(K)	F10.0	46-55	K = 4
	IBC(K)	I5	56-60	
	BBC(K)	F10.0	61-70	K = 5
	IBC(K)	I5	71-75	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	BBC(K)	F10.0	.	K = NOQ
	IBC(K)	I5	.	
4	NOBRK	I5	1-5	No. of values and times.
5	BCT(K)	F10.0	1-10	Value of broken lin. appx.
	T(K)	F10.0	11-20	Time at breaks (days); K = 1
	BCT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	BCT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	BCT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	BCT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	

ORGANIZATION OF RECORDS:

|1|2| |3|(NOBC(K)/5)|3| |4| |5|(NOBRK(K)/4)|5|

Sequence of Records for "E" Card Groups:

|E1, E2, or E3| |E1, E2, or E3|...|E1, E2, or E3|

NOSYS

DATA GROUP E.3

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IBCOP(K)	I5	1-5	Data input options.
	NOBC(K)	I5	6-10	No. of boundary conditions.
	TITLE	5A4	61-80	"E: Boundary Concentrations".
2	SCALB	E10.3	1-10	Scale factor.
	CONVB	E10.3	11-20	Units conversion factor.
3	IBC(I)	I5	1-5	Boundary segment number.
	NOBRK(I)	I5	6-10	No. of values and times.
4	BCT(K)	F10.0	1-10	Value of broken lin. appx.
	T(K)	F10.0	11-20	Time at breaks (days); K = 1
	BCT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	BCT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	BCT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	BCT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	

ORGANIZATION OF RECORDS:

$$\boxed{1}\quad \boxed{2}\quad \underbrace{\boxed{3}\ \ \boxed{4}\,\boxed{(NOBRK/4)}\,\boxed{4}\ \ \boxed{3}\ \ \boxed{4}\,\boxed{(NOBRK/4)}\,\boxed{4}\ \ \ldots\ \ \boxed{3}\ \ \boxed{4}\,\boxed{(NOBRK/4)}\,\boxed{4}}_{NOBC(K)}$$

Sequence of Records for "E" Card Groups:

$$\underbrace{\boxed{E1,\ E2,\ or\ E3}\ \ \boxed{E1,\ E2,\ or\ E3}\ \ldots\ \boxed{E1,\ E2,\ or\ E3}}_{NOSYS}$$

DATA GROUP F.1

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IWKOP(ISYS)	I5	1-5	Option number = 1
	NOWK(ISYS)	I5	6-10	Number of forcing functions.
	LOPT	I5	11-15	Indicates runoff loads in F.4
	TITLE	5A4	61-80	"F: Waste Loads".
2	SCALW	E10.3	1-10	Scale factor for forcing func
	CONVW	E10.3	11-20	Units conversion factor.
3	BWK(K)	F10.0	1-10	Forcing function; K = 1
	IWC(K)	I5	11-15	Segment number
	BWC(K)	F10.0	16-25	K = 2
	IWC(K)	I5	26-30	
	BWC(K)	F10.0	31-40	K = 3
	IWC(K)	I5	41-45	
	BWC(K)	F10.0	46-55	K = 4
	IWC(K)	I5	56-60	
	BWC(K)	F10.0	61-70	K = 5
	IWC(K)	I5	71-75	
	. . .	. . .	. . .	. . .
	BWC(K)	F10.0	.	K = NOWK
	IWC(K)	I5	.	

ORGANIZATION OF RECORDS for F.1:

|1|2| |3|(NOWK/5)|3|

DATA GROUP F.2

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IWKOP(ISYS)	I5	1-5	Option number = 2
	NOWK(ISYS)	I5	6-10	Number of forcing functions.
	LOPT	I5	11-15	Indicates runoff loads in F.4
	TITLE	5A4	61-80	"F: Waste Loads".
2	SCALW	E10.3	1-10	Scale factor for forcing func
	CONVW	E10.3	11-20	Units conversion factor.
3	BWK(K)	F10.0	1-10	Ratio of forcing function
	IWC(K)	I5	11-15	Segment number; K = 1
	BWC(K)	F10.0	16-25	K = 2
	IWC(K)	I5	26-30	
	BWC(K)	F10.0	31-40	K = 3
	IWC(K)	I5	41-45	
	BWC(K)	F10.0	46-55	K = 4
	IWC(K)	I5	56-60	
	BWC(K)	F10.0	61-70	K = 5
	IWC(K)	I5	71-75	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	BWC(K)	F10.0	.	K = NOWK
	IWC(K)	I5	.	
4	NOBRK	I5	1-5	No. of values and times.
5	WKT(K)	F10.0	1-10	Value of forcing functions.
	T(K)	F10.0	11-20	Time in days; K = 1
	WKT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	WKT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	WKT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	WKT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	

ORGANIZATION OF RECORDS:

|1|2| |3|(NOWK/3)|3| |4| |5|(NOBRK(K)/4)|5|

Sequence of Records for "F" Card Groups:

|F1, F2, or F3| |F1, F2, or F3|...|F1, F2, or F3|

NOSYS

DATA GROUP F.3

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	IWKOP(ISYS)	I5	1-5	Option number = 3
	NOWK(ISYS)	I5	6-10	Number of forcing functions.
	LOPT	I5	11-15	Indicates runoff loads in F.4
	TITLE	5A4	61-80	"F: Waste Loads".
2	SCALW	E10.3	1-10	Scale factor for forcing func
	CONVW	E10.3	11-20	Units conversion factor.
3	IWK(K)	I5	1-5	Segment number.
	NOBRK(K)	I5	6-10	Number of breaks.
4	WKT(K)	F10.0	1-10	Value of forcing functions.
	T(K)	F10.0	11-20	Time in days; K = 1
	WKT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	WKT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	WKT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	WKT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	

ORGANIZATION OF RECORDS:

$$\boxed{1}\ \boxed{2}\ \underbrace{\boxed{3}\ \boxed{4\,|\,(NOBRK/4)\,|\,4}\ \boxed{3}\ \boxed{4\,|\,(NOBRK/4)\,|\,4}\ \ldots\ \boxed{3}\ \boxed{4\,|\,(NOBRK/4)\,|\,4}}_{NOWK}$$

Sequence of Records for "F" Card Groups:

$$\underbrace{\boxed{F1,\ F2,\ or\ F3}\ \boxed{F1,\ F2,\ or\ F3}\ldots\boxed{F1,\ F2,\ or\ F3}}_{NOSYS}$$

DATA GROUP F.4

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NOWKS	I5	1-5	Number of runoff loads.
	NPSDAY	I5	6-10	Time in runoff file corresponding to TZERO.
2	SCALN	F10.0	1-10	Scale factor for runoff loads
	CONVN	F10.0	11-20	Units conversion factor.
3	INPS(J)	I5	1-5	Runoff segment 1.
	INPS(J)	I5	6-10	Runoff segment 2.
	INPS(J)	I5	11-15	Runoff segment 3.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	INPS(J)	I5	75-80	Runoff segment 16.
4	KT1	F5	1-5	Initial runoff print day.
	KT2	F5	6-10	Final runoff print day.
	KPRT(I)	F5	11-15	Indicates print system 1.
	KPRT(I)	F5	16-20	Indicates print system 2.
	KPRT(I)	F5	21-25	Indicates print system 3.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	KPRT(I)	F5	75-80	Indicates print system 14.

ORGANIZATION OF RECORDS:

|1| |2| |3|(NOWKS/16)|3| |4|

DATA GROUP G

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NOPAM	I5	1-10	No. of parameters required.
	TITLE	5A4	61-80	"G: Environmental Parameters".
2	SCALP(K)	E10.3	1-10	Scale factor group K.
	SCALP(K)	E10.3	11-20	K = 2
	SCALP(K)	E10.3	21-30	K = 3
	SCALP(K)	E10.3	31-40	K = 4
	SCALP(K)	E10.3	41-50	K = 5
	SCALP(K)	E10.3	51-60	K = 6
	SCALP(K)	E10.3	61-70	K = 7
	SCALP(K)	E10.0	71-80	K = 8
	.	.	.	.
	.	.	.	.
	.	.	.	.
	SCALP(K)	E10.3	71-80	K = NOPAM
3	ANAME(K)	A5	1-5	Opt. descriptive name; K = 1
	PARAM(ISEG,K)	F10.0	6-15	Value of parameter ANAME(K).
	ANAME(K)	A5	16-20	K = 2
	PARAM(ISEG,K)	F10.0	21-30	
	ANAME(K)	A5	31-35	K = 3
	PARAM(ISEG,K)	F10.0	36-45	
	ANAME(K)	A5	56-50	K = 4
	PARAM(ISEG,K)	F10.0	51-60	
	ANAME(K)	A5	61-65	K = 5
	PARAM(ISEG,K)	F10.0	66-75	
	.	.	.	.
	.	.	.	.
	ANAME(K)	F10.0	.	K = NOPAM
	PARAM(ISEG,K)	F10.0	.	

ORGANIZATION OF RECORDS:

$\boxed{1}$ $\boxed{2}\boxed{\text{(NOPAM/8)}}\boxed{2}$ $\boxed{3}\boxed{\text{(NOPAM/5)}}\boxed{3}$

DATA GROUP H

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NCONS	I5	1-10	No. of constants required.
	TITLE	5A4	61-80	"H: Chemical Constants".
2	ANAME(K)	A5	1-5	Opt. descriptive name; K = 1
	CONST(K)	F10.0	6-15	Value of constant ANAME(K).
	ANAME(K)	A5	16-20	K = 2
	CONST(K)	F10.0	21-30	
	ANAME(K)	A5	31-35	K = 3
	CONST(K)	F10.0	36-45	
	ANAME(K)	A5	56-50	K = 4
	CONST(K)	F10.0	51-60	
	ANAME(K)	A5	61-65	K = 5
	CONST(K)	F10.0	66-75	
	.	.	.	.
	.	.	.	.
	ANAME(K)	F10.0	.	K = NOPAM
	CONST(K)	F10.0	.	

ORGANIZATION OF RECORDS:

|1| |2 (NCONS/5) 2|

DATA GROUP I

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NFUNC	I5	1-5	No. time functions required.
	TITLE	5A4	61-80	"I: Time Functions".
2	ANAME(I)	A5	1-5	Optional descriptive name.
	NOBRK(I)	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1
	VALT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	VALT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	VALT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	VALT(K)	F10.0	.	K = NOBRK
	T(K)	F10.0	.	

ORGANIZATION OF RECORDS:

|1| |2| |3 (NOBRK/4) 3| |2| |3 (NOBRK/4) 3| . . . |2| |3 (NOBRK/4) 3|

NFUNC

DATA GROUP J

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	TITLE	5A4	61-80	"J: Initial Concentrations".
2	ANAME(K)	A5	1-5	Opt. descriptive name; K = 1
	C(ISYS,K)	F10.0	6-15	Value of constant ANAME(K).
	ANAME(K)	A5	16-20	K = 2
	C(ISYS,K)	F10.0	21-30	
	ANAME(K)	A5	31-35	K = 3
	C(ISYS,K)	F10.0	36-45	
	ANAME(K)	A5	56-50	K = 4
	C(ISYS,K)	F10.0	51-60	
	ANAME(K)	A5	61-65	K = 5
	C(ISYS,K)	F10.0	66-75	
	.	.	.	.
	.	.	.	.
	ANAME(K)	F10.0	.	K = NOSEG
	C(ISYS,K)	F10.0	.	

ORGANIZATION OF RECORDS:

|1| |2|NOSEG/4|2| |2|NOSEG/4|2|...|2|NOSEG/4|2|

NOSYS

DATA GROUP K

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	CMAX(K)	F10.0	1-10	Maximum concentration for
	CMAX(K)	F10.0	11-20	systems 1 through NOSYS.
	CMAX(K)	F10.0	21-30	
	.	.	.	.
	.	.	.	.
	.	.	.	.
	CMAX(K)	F10.0	71-80	K = NOSYS
2	CMIN(K)	F10.0	1-10	K = 1 Minimum concentrations
	CMIN(K)	F10.0	11-20	K = 2 for systems 1 through
	CMIN(K)	F10.0	21-30	K = 3 NOSYS
	.	.	.	.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	CMIN(K)	F10.0	71-80	K = NOSYS

ORGANIZATION OF RECORDS:

|1|(NOSYS/8)|1| |2|(NOSYS/8)|2|

DATA GROUP L.1

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NPRINT	I20	1-20	Number of print intervals.
	TITLE	5A4	61-80	"L: Sys-Seg display control".
2	PRINT(I)	F10.0	1-10	Print interval (day).
	TPRINT(I)	F10.0	11-20	Final day for application of PRINT(I) (day).
	.	.	.	
	.	.	.	
	.	.	.	
	PRINT(I)	F10.0	61-70	Print interval (day).
	TPRINT(I)	F10.0	71-80	
3	ISYS(1)	I3	1-3	System segment
	ISEG(1)	I3	4-6	
	ISYS(2)	I3	7-9	
	ISEG(2)	I3	10-12	
	.	.	13-15	
	.	.	16-18	
	.	.	19-21	
	.	.	22-24	
	.	.	25-27	
	.	.	28-30	
	.	.	31-33	
	.	.	34-36	
	.	.	37-39	
	.	.	40-42	
	ISYS(8)	I3	43-45	
	ISEG(8)	I3	46-48	

ORGANIZATION OF RECORDS:

|1| |2|(NPRINT/4)|2| |3|

DATA GROUP L.2

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NPRINT	I20	1-20	Number of print intervals.
	TITLE	5A4	61-80	"L: Sys-Seg display control".
2	PRINT(I)	F10.0	1-10	Print interval (day).
	TPRINT(I)	F10.0	11-20	Final time for application of PRINT(I) (day).
	.	.	.	
	.	.	.	
	.	.	.	
	PRINT (NPRINT)	F10.0	61-70	
	TPRINT(I)	F10.0	71-80	
3	IMCHK (=0)	I3	1-3	Mass check for system SYS.
	MSYS	I3	4-6	System number.

ORGANIZATION OF RECORDS:

|1| |2|(NPRINT/4)|2| |3|

DATA GROUP M

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	INTYP	I2	1-2	Integration option.
	NEGSLN	I2	3-4	Negative solution option.
	ADFAC	F6.0	5-10	Advection factor.
	TITLE	5A4	61-80	"M: Integration Control".
2	SCALT	E10.4	1-10	Time warp scale factor.
	TZERO	E10.4	11-20	Starting simulation time.
3	NOSTEP	I5	1-5	No. integration step sizes.
4	DT(K)	F10.0	1-10	Integration step size; K = 1
	TIME(K)	F10.0	11-20	Time DT(K) will be used (day).
	DT(K)	F10.0	21-30	K = 2
	TIME(K)	F10.0	31-40	
	DT(K)	F10.0	41-50	K = 3
	TIME(K)	F10.0	51-60	
	DT(K)	F10.0	61-70	K = 4
	TIME(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	DT(K)	F10.0	.	K = NOSTEP
	TIME(K)	F10.0	.	

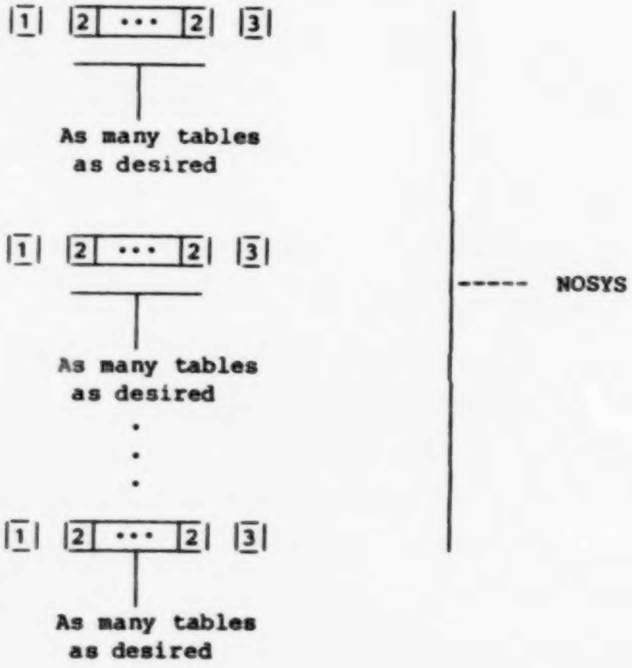
ORGANIZATION OF RECORDS:

$\boxed{1}$ $\boxed{2}$ $\boxed{3}$ $\boxed{4}\boxed{\text{(NOSTEP/4)}}\boxed{4}$

DATA GROUP N

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	ANAME(1)	A8	1-8	Descriptive name for display variable K.
	ANAME(2)	A8	8-16	
	ANAME(3)	A8	17-24	
	ANAME(4)	A8	25-32	
	ANAME(5)	A8	33-40	
	ANAME(6)	A8	41-48	
	ANAME(7)	A8	49-56	
	ANAME(8)	A8	57-64	
	TITLE	4A4	65-80	"N: Print Tablesd".
2	VARNO	I3	1-3	Number of desired variable.
	SEG(K)	I3	4-6	Segment no. to be displayed. (Variable number and segment number.)
	SEB(K)	I3	7-9	
	SEG(K)	I3	10-12	
	SEG(K)	I3	13-16	
	SEG(K)	I3	16-18	
	SEG(K)	I3	19-21	
	SEG(K)	I3	22-24	
	SEG(K)	I3	25-27	
3	Blank		1-80	

ORGANIZATION OF RECORDS:

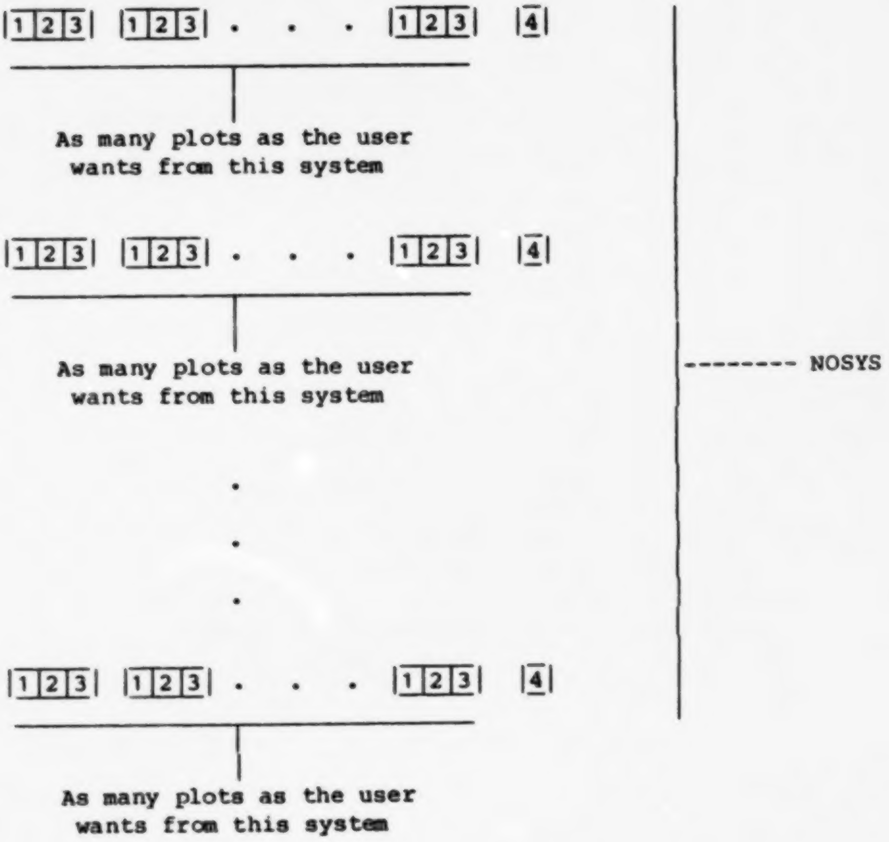

1
2 ··· 2
3
As many tables as desired
1
2 ··· 2
3
As many tables as desired

NOSYS
1
2 ··· 2
3
As many tables as desired

DATA GROUP O

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NSPLT	I2	1-2	No. segments to be plotted.
	VARNO	I2	3-4	Position of desired variable.
	TITLE	5A4	61-80	"O: Time PLots".
2	PMIN	F10.0	1-10	Minimum value for this plot.
	PMAX	F10.0	11-20	Maximum value for this plot.
3	SEG(1)	I3	1-3	Segment no. to be plotted.
	SEG(2)	I3	4-6	
	.	.	.	
	.	.	.	
	SEG(NSPLIT)	I3	.	
4	(blank)		1-80	Blank

ORGANIZATION OF RECORDS:



1 2 3
4
As many plots as the user wants from this system
As many plots as the user wants from this system
NOSYS
As many plots as the user wants from this system

DATA GROUP P

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	RM1	F5.0	1-5	Minimum river mile value.
	RM2	F5.0	6-10	Maximum river mile value.
	TITLE	5A4	61-80	"P: Spatial Plots".
2	SEG(K)	I5	1-5	Segment number; K = 1
	RM(K)	F5.0	6-10	River mile value for SEG(K).
	SEG(K)	I5	11-15	K = 2
	RM(K)	F5.0	16-20	
	SEG(K)	I5	21-25	K = 3
	RM(K)	F5.0	26-30	
	SEG(K)	I5	71-75	K = 4
	RM(K)	F5.0	76-80	
	.	.	.	.
	.	.	.	.
	SEG(K)	I5	.	K = NOSEG
	RM(K)	F5.0	.	
3	MXTIM	I5	1-5	No. of time selections.
	IVAR	I5	6-10	Position of desired variable.
	YSTR	F5.0	11-15	Minimum values.
	YSTP	F5.0	16-20	Maximum values.
	SYSOPT	I5	21-25	System number.
	OVRLAY	I5	26-30	Flag to cause plot overlay.
	TITL1	40A	31-70	Title for plot.
4	TIM(1)	F5.0	1-5	Time selections for this plot
	TIM(2)	F5.0	6-10	
	TIM(3)	F5.0	11-15	
	TIM(4)	F5.0	16-20	
	TIM(5)	F5.0	21-25	
	SYMTAB(1)	A1	26	Plot symbols.
	SYMTAB(2)	A1	27	
	SYMTAB(3)	A1	28	
	SYMTAB(4)	A1	29	
	SYMTAB(5)	A1	30	
5	FLAG	I5	1-5	Flag to indicate obs. data.
	IUNIT	I5	6-10	Unit device number = 5.
	YSTR	F5.0	11-15	Minimum value.
	YSTP	F5.0	16-20	Maximum value.
	NOOBS	I5	21-25	No. obs. data points.
	OVRLAY	I5	26-30	Flag to cause plot overlay.
	TITL1	40A	31-70	Title for this plot.
	OBSSYM	1A	71	Plot symbol.

DATA GROUP P (Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
6	RIVMIL(K)	F10.0	1-10	River mile location; K = 1
	VALUE(K)	F10.0	11-20	Obs.val. of var. RIVMIL(K)
	RIVMIL(K)	F10.0	21-30	K = 2
	VALUE(K)	F10.0	31-40	
	RIVMIL(K)	F10.0	41-50	K = 3
	VALUE(K)	F10.0	51-60	
	RIVMIL(K)	F10.0	61-70	K = 4
	VALUE(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	RIVMIL(K)	F10.0		K = 5
	VALUE(K)			
7	FMT	20A4	1-80	Format specification

ORGANIZATION OF RECORDS FOR DATA GROUP P

|1| |2|(NOSEG/8)|2| |3|4| or |5|6|(NOOBS/4)|6| or |5|7|

|3|4| or |5|6|(NOOBS/4)|6| or |5|7|

.

.

.

|3|4| or |5|6|(NOOBS/4)|6| or |5|7|

---As many spatial plots as the user wants

2.3.4 WASP3 Variable Definitions

The following list defines the variables contained in the WASP3 COMMON. COMMON is used by the Basic Water Quality Model, WASP3, as the vehicle to pass information from subroutine to subroutine within the program. The following is alphabetical listing of the COMMON variables, their definitions and units, and location description.

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
ADFAC	CPRINT	Advection factor (0-0.5).	unit-less
AIMASS	MASS	Total mass of designated constituent advected in.	kg
AOMASS	MASS	Total mass of designated constituent advected out.	kg
BBC(SY,BC)	REAL	Boundary condition intercepts.	mg/L
BFUNC(TF)	REAL	Intercepts for the time variable functions required for the WASPS kinetic subroutine.	vari-able
BQ(S2)	REAL	Advective flow intercepts	MCF/day
BR(S2)	REAL	Exchange coefficient intercepts.	MCF/day
BVOL(SG)*	REAL	Segment volumes.	MCF
BWK(SY,WK)	REAL	Forcing function intercepts.	lb/day
C(SY,SG)	REAL	State variable or water quality concentration array.	mg/L
CD(SY,SG)	REAL	Derivative array.	$\frac{mg}{L} \cdot \frac{MCF}{day}$
CMAX(20)	REAL	Stability criteria vector. The vector contains the maximum allowable segment concentration for each system. If any system (usually because the integration stepsize is too large), the simulation is terminated.	mg/L
CMIN(SY)*	REAL	Not used in current version of WASP (although user must include in his input data check).	unit-less
CONST(CX)*	REAL	Constants for use in the WASPB kinetic subroutine.	vari-able

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
DAY	DAYIND	Current day.	day
DQTIME	DAYIND	Time until next specified flow in piecewise linear function.	day
DRTIME	DAYIND	Time until next specified exchange in piecewise linear function.	day
DT	REAL	Current integration time step.	days
DTIME	DUMP	Array that stores print times for tables.	unitless
DWKTIM	DAYIND	Time until next specified load in piecewise linear function.	unitless
DVAR(MY,SY)	DUMP	Array that stores tables of constituents for printing and plotting.	unitless
DVOL(MP,S6)	DUMP	Array that stores tables of volumes.	unitless
FILE30(MB, M30)	SCRTCH	Array that stores boundary conditions.	unitless
FILE50(MB, M50)	SCRTCH	Array that stores loads.	unitless
FILE70(MB, M70)	SCRTCH	Array that stores exchanges.	unitless
FILE72(MB, M72)	SCRTCH	Array that stores advective flows.	unitless
FILE73(MB, M73)	SCRTCH	Array that stores kinetic time functions.	unitless
FILE75 (M75,1)	SCRTCH	Array that stores time steps.	unitless
FILE80(SY, 20)	SCRTCH	Array that stores display variable names.	unitless
IBC(SY,BC)*	INTGR	Contains the segment numbers for which boundary conditions have been specified.	unitless
IBOCP(SY)*	INTGR	User selected forcing function input option for each system. IBCOP(ISYS) flags the boundary conditions for system ISYS as	unitless

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
		being constant in time (IBCOP(ISYS)=1) or time-variable (IBCOP(ISYS)= 2,3).	
IDFRC(19)	INTGR	Used only in the DEC-PDP version as the record address pointers for the direct access dump files.Not needed for the IBM 370 version because sequential files are used.	unitless
IDISK	INTGR	When checked by the user in the kinetic subroutine,WASPB, IDISK acts as internal program indicator that informs the user when a print interval has been reached, permitting the user to write the current state variables or segment concentrations to auxiliary storage (disk). Normally IDISK equals zero, but at a print interval it is exter nally set to one; must be reset by the user before exiting the WASPB.	unitless
IDUMP(8,2)	INTGR	System - segment combinations to be printed out during the integration procedure.	unitless
IN	INTGR	Device number for reading input data.	unitless
INITB	INTGR	Internal program indicator that permits the user to perform initialization or to execute special code upon initial entry to the WASPB kinetic subroutine. Initially equal to zero, INITB must be reset by the user in WASPB.	unitless
INPS(WK)	NPSCOM	Input segment for nonpoint source load.	unitless
IPRNT	INTGR	Not currently used.	
IQ(S2)*, JQ(S2)*	INTGR	Contain the segment numbers between which advective flow is to take place. If the advective flow is positive, then JQ will contain the upstream segment number (from which flow is leaving) and IQ will contain the downstream segment number (to which flow will go). If, however, the advective flow is negative, then JQ, will be considered the downstream segment (flow to) and IQ will be considered the upstream segment (flow from).	unitless

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
IR(S2)*, JR(S2)*	INTGR	Contain the segment numbers between which change is to take place.	unitless
IREC	INTGR	Internal counter used to keep track of the number ofprint intervals generated during the course of the simulation.	unitless
ISIM*	INTGR	Simulation type - currently only time variable is permitted.	unitless
ISYS	INTGR	System currently having its derivatives evaluated.	unitless
ITCHCK	INTGR	Not used in current version of WASP.	
ITIMB(SY, BC)	INTGR	Used as a breakpoint counter for obtaining correct slope and intercept values for time-variable boundary conditions.	unitless
ITIMF(TF)	INTGR	Used as a breakpoint counter for obtaining correct slope and intercept values for the time-variable functions required by the WASPB kinetic sub- routine.	unitless
ITIMQ	INTGR	Used as a breakpoint counter for obtaining correct slope and intercept values for time-variable advective flows.	unitless
ITIMR	INTGR	Used as a breakpoint counter for obtaining correct slope and intercept values for the time-variable exchange coefficients.	unitless
ITIMV	INTGR	Not used in current version of WASP.	
ITIMW(SY, WK)	INTGR	Used as a breakpoint counter for obtaining correct slope and intercept values for time-variable forcing function.	unitless
IVOPT*	INTGR	User selected volume input option. 1 = constant volumes; 2,3 = volumes adjusted for flow continuity.	unitless
IWK(SY,WK)*	INTGR	Contains the segment number for which forcing functions have been specified (i.e., receiving water segments for waste loads).	unitless

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
IWKOP(SY)*	INTGR	User selected forcing functions input option for each system. IWKOP*ISYS) flags the forcing functions for system ISYS as being constant in time (IWKOP(ISYS)=1 or time-variable (IWKOP(ISYS)= 2,3).	unitless
LDAY	DAYIND	Current day counter.	day
LISTC*	INTGR	User selected option to print forcing function (waste load), kinetic constants, segment para- meters and miscellaneous kinetic time functions, and initial condition input data.	unitless
LISTG*	INTGR	User selected option to print exchange coefficient, segment volume, advective flow and boundary condition input data.	unitless
LOPT	NPSCOM	Option to read in nonpoint source loads.	unitless
MBC(SY,BC)	REAL	Boundary condition slopes.	$\frac{mg}{L \cdot day}$
MFUNC(TF)	REAL	Slopes for the time-variable functions required for the WASPB kinetic subroutines.	variable
MQ(S2)	REAL	Advective flow slopes.	$\frac{MCF}{day.day}$
MR(S2)	REAL	Exchange coefficient slopes.	$\frac{MCF}{day.day}$
MVOL(SG)	REAL	Not used in current version of WASP.	
MXDMP	INTGR	Blocking factor or the maximum number of variables saved per segment at each print.	unitless
MXITER	INTGR	Not used in current version of WASP.	unitless
MXSEG	PDP	Maximum number of segments.	unitless
MXSYS	PDP	Maximum number of systems.	unitless
NBCPSY	INTGR	Maximum number of forcing functions (waste loads) permitted per system; set for a particular WASP configuration in subroutine WASP1.	unitless

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
NBRK30(BC)	SCRTCH	Array that stores number of steps in boundary functions.	unitless
NBRK50(WK)	SCRTCH	Array that stores number of steps in load functions.	unitless
NBRK70(1)	SCRTCH	Array that stores number of steps in exchange functions.	unitless
NBRK72(1)	SCRTCH	Array that stores number of steps in flow functions.	unitless
NBRK73(TF)	SCRTCH	Array that stores number of steps in kinetic functions.	unitless
NBRK75(1)	SCRTCH	Array that stores number of steps in time step functions.	unitless
NCONS*	INTGR	Number of constants (for use in the WASPB kinetic subroutine) read.	unitless
NDAY	DAYIND	Integer set equal to current simulation.	day
NEGSLN*	INTGR	Indicates whether the user has chosen to permit to compute negative water quality concentrations. (Example: permit negative D.O. deficit, i.e., supersaturation). NEGSLN normally equal zero, will equal one, if user chooses to permit negative solutions.	unitless
NEWDAY	DAYIND	Integer equal to one each time of a new simulation.	day
NFUNC*	INTGR	Number of time variable functions (for use in the WASPB kinetic subroutine) read.	unitless
NFUNT(TF)	REAL	Used if time variable functions (approximated as piecewise linear functions of time) have been read for use in the WASPB kinetic subroutine. NFUNT will contain the time at which the next break in the piecewise linear functions will occur, at which point it will be necessary to obtain new slopes (MFUNC) and intercepts (BFUNC).	day

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
NOBC(SY)*	INTGR	Number of boundary conditions read for each system.	unitless
NOPAM*	INTGR	Number of segment parameters (for use in the WASPB kinetic subroutine) read.	unitless
NOSYS*	INTGR	Number of systems or water quality constituents in the user's model.	unitless
NOV*	INTGR	Number of volumes (normally NOV equals NOSEG).	unitless
NOWK(SY)*	INTGR	Number of forcing functions read for each system.	unitless
NOWKS	NPSCOM	Number of nonpoint source loads used in this simulation.	unitless
NPSWK(SY, WK)	NPSCOM	Nonpoint source load.	lb/day
NQT	REAL	Used if the exchange coefficients are time-variable (apppro ximated by a piecewise linear functions of time). NQT will contain the time at which the next break in the piecewise linear functions will occur, at which point it will be necessary to obtain new slopes (MRC) and intercepts (BR).	
NRT	REAL	Used if the exchange coefficients are time-variable (approximated by a piecewise linear functions of time). NRT will contain the time at which the next break in the piecewise linear functions will occur, at which point it will be neces sary to obtain new slopes (MRC) and intercepts (BR).	
NVOLT	REAL	Not used in the current version of WASP.	
NWKPSY	INTGR	Maximum number of forcing functions (waste loads) permitted per system; set for a particular WASP configuration in subroutine WASP1.	unitless
NWKS	NPSCOM	Number of nonpoint source loads on file.	unitless

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
NWKT(SY,WK)	REAL	Used if the forcing functions for a system are time-variable (approximated by a piecewise linear function of time). NWKT(ISYS) will contain the time at which the next break in the piecewise linear functions, for system ISYS, will occur, at which point it will be necessary to obtain new slopes (MWK) and intercepts (BWK) for system ISYS.	day
OMEGA	REAL	Not used in current version of WASP.	
OUT	INTGR	Device number for printer output.	unitless
PARAM(SG, PR)*	REAL	Segment parameters for use in the WASPB kinetic subroutine.	variable
PRINT(20)	CPRINT	Print interval.	day
PRNT*	REAL	Print interval.	day
QBY(SY)*	INTGR	User selected advective transport indicators. If a user wishes, he may by-pass advective transport for a particular system, ISYS, by setting IBY(ISYS) appropriately. (Example: if a user had incorporated rooted aquatic plants in his model, he would not wish to have them transported via flow).	unitless
RBY(SY)*	INTEGR	User selected exchange transport by-pass indicaters. If a user wishes, he may bypass exchange transport for a particualr system, ISYS, by setting RBY(ISYS) appropriately. (Example: if a user had incorporated rooted aquatic plants in his model, he would not wish to have them "disperse").	unitless
RIMASS	MASS	Total mass of designated constituent dispersed in.	kg
ROMASS	MASS	Total mass of designated constituent dispersed out.	kg
SCALT(*)	REAL	Time scale factor. Not used in current version of WASP.	

VARIABLE	FOUND IN COMMON	DEFINITION	UNITS
SYSBY(SY)*	INTGR	User selected system by-pass indicators. If a user wishes he may choose to by-pass computations for a particular system (or systems), ISYS, for a simulation run by setting SYSBY (ISYS) appropiately.	unitless
TEND	REAL	Ending time for use of the current integration step size. For single integration stepsize input this will be the total simulation time. For multiple integration stepsize histories, when TIME equals TEND, a new integration step size will be chosen and TEND reset.	day
TIME	REAL	Current simulation time.	day
TPRINT	CPRINT	Time for next printout.	day
TPRINT(20)	CPRINT	Time through which print interval is used.	day
TZERO*	REAL	User selected time for start of simulation. If for example a user's input data for model was up such that time zero was January 1, a user may skip computations for January and February and start March 1 by setting TZERO (on input).	day
XBMASS	MASS	Total mass of designated constituent buried or volatilized.	kg
XKMASS	MASS	Total mass of designated constituent transformed.	kg
XLMASS	MASS	Total mass of designated constituent loaded in.	kg
XMASS0	MASS	Total mass of designated constituent in network.	kg

2.4 THE EUTROPHICATION MODEL

2.4.1 Introduction

EUTRWASP requires the same input format as the basic WASP3 model. This format is explained in detail in Section 2.3. This section describes variables needed specifically for EUTRWASP. Elaborations on WASP3 occur only in Data Groups G, H, and I. Records or variables within a record that are not mentioned here remain the same as described in Section 2.3.

As mentioned in Table 19, the 8 systems for eutrophication modeling are: ammonia nitrogen, nitrate nitrogen, ortho-phosphate phosphorus, phytoplankton carbon, carbonaceous BOD, dissolved oxygen, organic nitrogen, and organic phosphorus. In data groups E, F, J, N, and O, input will be repeated 8 times, once for each system.

2.4.2 EUTRWASP Data Descriptions

2.4.2.1 DATA GROUP A: Model Identification and System Bypass Option--

Record 1--Model Identification

NOSYS = 8 for EUTRWASP.

2.4.2.2 DATA GROUP B: Exchange Coefficients--

No changes.

2.4.2.3 DATA GROUP C: Volumes--

No changes.

2.4.2.4 DATA GROUP D: Flows--

No changes.

2.4.2.5 DATA GROUP E: Boundary Concentrations--

No changes. Input is repeated 8 times, once for each system.

2.4.2.6 DATA GROUP F: Waste Loads--

No changes. Input is repeated 8 times, once for each system.

2.4.2.7 DATA GROUP G: Environmental Parameters--

Record 1--Number of Parameters

NOPAM = 13 for eutrophication

TITLE = name of data group

Record 2--Scale Factors for Parameters

SCALP(K) = scale factor for parameter K.

K = 1, 13

Record 3--Segment Parameters

ANAME(K) = an optional one to five alpha-numeric character descriptive name for parameter PARAM(ISEG,K).

PARAM(ISEG,K) = the value of parameter ANAME(K) in segment ISEG.

K = 1, NOPAM

ISEG = 1, NOSEG

Listed below are the 13 parameters required for eutrophication. Enter these variables and their respective values in place of ANAME (K) and PARAM (ISEG,K).

K	PARAM(ISEG,K)	ANAME (K)	Definition and Units
1	DEPTH(ISEG,1)	DEPTH	Depth of segment (ft).
2	TYPEE(ISEG,2)	TYPEE	Flag designating segment type: 1 = surface water 2 = subsurface water 3 = bed
3	BOTSG(ISEG,3)	BOTSG	Segment number of segment below current segment.
4	VELSGM(ISEG,4)	VELSGM	Water velocity in segment ISEG, ft/sec.
5	TMPSG(ISEG,5)	TMPSG	Segment temperature multiplier (°C). TMPSG varies over space and can be either actual temperature or a normalized function, depending on the definition of TEMP. TMPSG(ISEG)*TEMP (TMPFN(ISEG))= STP, the temperature of segment ISEG.

K	PARAM(ISEG,K)	ANAME (K)	Definition and Units
6	TMPFN(ISEG,6)	TMPFN	Flag designating the time--variable temperature function to be used for segment ISEG. The four temperature functions, supplied by the user, are defined in data group I (Section 2.4.4). = 1, TEMP(1) = 2, TEMP(2) = 3, TEMP(3) = 4, TEMP(4)
7	KESG(ISEG,7)	KESG	Segment extinction coefficient multiplier (ft^{-2}). KESG varies over space and can be either an actual extinction coefficient or a normalized function, depending on the definition of KE. KESG(ISEG) * KE(KEFN(ISEG)) = KESG(ISEG). KE(KEFN(ISEG)) = K_e, the extinction coefficient for segment ISEG.
8	KEFN(ISEG,8)	KEFN	Flag designating the time variable extinction coefficient (KE) to be used for segment ISEG. The five extinction coefficients available are defined in data Group I (Section 2.4.2.9). = 1, KE(1) = 2, KE(2) = 3, KE(3) = 4, KE(4) = 5, KE(5)
9	EDIF(ISEG,9)	EDIF	Dispersion coefficient for exchange of dissolved chemical between ISEG and IBOT; converted to dispersive volume internally. (cm^2/day = million ft^3/day).
10	SOD1D(ISEG,10)	SOD1D	Sediment oxygen demand; one dimensional networks only (g/m^2/day).
11	FPIPWC(ISEG,11)	FPIPW	Spatially variable fraction of inorganic PO_4 sorbed to particulates, and subject to settling.
12	FNH4(ISEG,12)	FNH4	Average ammonium flux multiplier for segment; one-dimensional water column networks only.

K	PARAM(ISEG,K)	ANAME (K)	Definition and Units
13	FPO4(ISEG,13)	FPO4	Average phosphate flux multiplier for segment; one-dimensional water column networks only ($mg/m^2/day$).

ORGANIZATION OF RECORDS

Record 1 is input once in Data Group G, occupying one line. Record 2 has 13 entries, occupying two lines. Record 3 has 13 entries per segment. At five entries per line, each segment requires three lines.

2.4.2.8 DATA GROUP H: Constants--

VARIABLES

Record 1--Number of Constants

NCONS = 49 for eutrophication.

TITLE = Name of data group.

Record 2--Constants

ANAME(K) = an optional one to five alpha-numeric character descriptive name for constant CONST(K).

CONST(K) = the value of constant ANAME(K).

K = 1, 49

Listed below are the 49 constants required for eutrophication. Enter these variable names and their values, respectively, for ANAME(K) and CONST(K).

K	CONST(K)	ANAME(K)	Definition and Units
1	K1C	K1C	Saturated growth rate of phytoplankton (day^{-1}).
2	K1T	K1T	Temperature coefficient.
3	LGHTSW	LGHTS	Light formulation switch: = 0, use Dick Smith's (USGS) formulation = 1, use DiToro et al. (1971) formulation
4	PHIMX	PHIMX	Maximum quantum yield constant. Used only when LIGHTSW = 0, mgC/mole photons.

K	CONST(K)	ANAME(K)	Definition and Units
5	XKC	XKC	Chlorophyll extinction coefficient. Used only when LGHTSW = 0, $(\text{mg chla/m}^3)^{-1}/\text{m}$.
6	CCHL	CCHL	Carbon-to-chlorophyll ratio. Used only when LGHTSW = 1 (mg carbon/mg chla).
7	IS1	IS1	Saturation light intensity for phytoplankton. Used only when LGHTSW = 1 (Ly/day).
8	KMNG1	KMNG1	Nitrogen half-saturation constant for nitrogen for phytoplankton growth, which also affects ammonia preference, mg-N/L. NOTE: This affects ammonia preference: = 0, PNH3G1 = 1.0 = Large, PNH3G1 = $NH_3/(NH_3 + NO_3)$ NOTE: For standard models, use a large KMNG1.
9	KMPG1	KMPG1	Phosporous half-saturation constant for phytoplankton growth, mg PO_4-P/L.
10	K1RC	K1RC	Endogenous respiration rate of phytoplankton at 20°C, day^{-1}.
11	K1RT	K1RT	Temperature coefficient for phytoplankton growth.
12	K1D	K1D	Non-predatory phytoplankton death rate, day^{-1}.
13	KMPHYT	KMPHY	Half-saturation constant for phytoplankton, mg carbon/L. NOTE: As phytoplankton increases, mineralization of organic nitrogen and organic phosphorus increases. KMPHYT = small; little phytoplankton effect on mineralization = large; large concentration of phytoplankton needed to drive mineralization For standard models, use KMPHYT = 0.
14	PCRB	PCRB	Phosphorus-to-carbon ratio in phytoplankton, mg PO_4-P/mg.
15	NCRB	NCRB	Nitrogen-to-carbon ratio in phytoplankton, mg N/mg C.

K	CONST(K)	ANAME(K)	Definition and Units
16	OCRB	OCRB	Oxygen to carbon ratio in phytoplankton, mg O_2/mg C.
17	NUTLIM	NUTLIM	Nutrient limitation option. 0 = minimum 1 = multiplicative
18	DUMMY	Blank	Leave Blank.
19	FSBOD	FSBOD	Fraction of the carbonaceous biochemical oxygen demand that settles.
20	FSDP	FSOP	Fraction of the total non-living organic phosphorus that settles.
21	FSIP	FSIP	Spatially constant fraction of inorganic phosphorus that is sorbed to particulates and that settles. For spatial variability, use parameter FPIPWC and leave this constant blank (or zero).
22	FSON	FSON	Fraction of total non-living organic nitrogen that settles.
23	K58C	K58C	Mineralization rate of dissolved organic phosphorus, per day.
24	K58T	K58T	Temperature coefficient for K58C.
25	K1013C	1013C	Mineralization rate of dissolved organic nitrogen, per day.
26	K1013T	1320T	Temperature coefficient for K1013C.
27	K1320C	1320C	Nitrification rate at 20°C, per day.
28	K1320T	1320T	Temperature coefficient for K1320C.
29	K140C	K140C	Denitrification rate at 20°C, per day.
30	K140T	K140T	Temperature coefficient for K140C.
31	KNIT	KNIT	Half-saturation constant for nitrification-oxygen limitation, mg O_2/L.
32	KNO3	KNO3	Half-saturation constant for denitrification oxygen limitation, mgO_2/L.
33	KDC	KDC	BOD deoxygenation rate at 20°C, per day.

K	CONST(K)	ANAME(K)	Definition and Units
34	KDT	KDT	Temperature coefficient for carbonaceous deoxygenation in water column.
35	SVP1	SVP1	Settling velocity of phytoplankton, ft/day.
36	SVPP	SVPP	Settling velocity of particulate phosphorus, ft/day.
37	SVPN	SVPN	Settling velocity of particulate organic nitrogen, ft/day.
38	SVBOD	SVBOD	Settling velocity of particulate BOD fraction, ft/day.
39	SEDVEL	SEDVL	Sedimentation velocity, inches/year. Converts to ft/day internally.
40	SCOUR	SCOUR	Mean scour velocity, inches/year. NOTE: Gross deposition = SCOUR + SEDVEL.
41	KPZDC	KPZDC	Decomposition rate constant for phytoplankton in the sediment at 20°C, per day.
42	KPZDT	KPZDT	Temperature coefficient for decomposition of phytoplankton in sediment.
43	KOPDC	KOPDC	Decomposition rate of organic phosphorus in the sediment at 20°C, per day.
44	KOPDT	KOPDT	Temperature coefficient for decomposition of organic phosphorus in the sediment.
45	KONDC	KONDC	Decomposition rate constant for organic nitrogen in the sediment at 20°C, per day.
46	KONDT	KONDT	Temperature coefficient for decomposition of organic nitrogen in the sediment.
47	KDSC	KDSC	Decomposition rate of carbonaceous BOD in the sediment at 20°C, per day.
48	KDST	KDST	Temperature coefficient for carbonaceous deoxygenation in the sediment.
49	KBOD	KBOD	Half saturation constant for carbonaceous deoxygenation oxygen limitation.

ORGANIZATION OF RECORDS

Record 1 is entered once in Data Group H. Record 2 has 48 entries and uses 10 lines. Five entries (ANAME(K)-CONST(K) pairs) will fit per line.

2.4.2.9 DATA GROUP I: Miscellaneous Time Functions--

VARIABLES

Record 1--Number of Time Functions

NFUNC = 14 for eutrophication.

TITLE = Name of data group.

Record 2--Time Function Descriptions

ANAME(K) = an optional one to five alpha-numeric character descriptive name for the time function K.

NOBRK(K) = number of breaks used to describe the time function K.

K = 1, NFUNC

Listed below are the 14 time functions required for eutrophication. The variable names will be entered for ANAME(K) in Record 2 and their respective values will be entered in Record 3 for VALT(K) and T(K).

NOTE: Variables 1-4 are the four temperature-function options available for TMPFN in data Group G. Variables 8-12 are the five extinction coefficient options for KEFN, also in G.

K	ANAME(K)		VALT(K)
1	TEMP(1)	=	Time-variable temperature function 1. TEMP(K) can be either a normalized function or an actual temperature in °C, depending upon the definition of the parameter multiplier TMPSG(ISEG).
2	TEMP(2)	=	Time-variable temperature function 2, unitless or °C.
3	TEMP(3)	=	Time-variable temperature function 3, unitless or °C.
4	TEMP(4)	=	Time-variable temperature function 4, unitless or °C.

5 ITOT = Total daily solar radiation, langleys.

6 F = Fraction of daylight, days.

7 WIND = Wind velocity, feet/sec.

8 KE(1) = Time-variable extinction coefficient function 1. This can be either a normalized function or an actual extinction coefficient in ft^{-1}, depending upon the definition of the parameter multiplier KESG(ISEG).

9 KE(2) = Time-variable extinction coefficient function 2, unitless or ft^{-1}.

10 KE(3) = Time-variable extinction coefficient function 3, unitless or ft^{-1}.

11 KE(4) = Time-variable extinction coefficient function 4, unitless or ft^{-1}.

12 KE(5) = Time-variable extinction coefficient function 5, unitless or ft^{-1}.

13 TFNH4 = Normalized ammonium flux from bed, unitless.

14 TFPO4 = Normalized phosphate flux from bed, unitless.

Record 3--Time Functions

VALT(K) = value of the function at time T(K).

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK).

K = 1, NOBRK

ORGANIZATION OF RECORDS

Record 1 is entered once in Data Group I. Records 2 and 3, as a set, are repleated 14 times. Within each set, Record 2 is input once and Record 3 uses as many 80-space lines as needed to input NOBRK entries. Four entries (four VALK(K)-T(K) pairs) will fit on each 80-space line.

2.4.2.10 DATA GROUP J: Initial Concentrations--

No changes. Input is repeated 8 times, once for each system.

2.4.2.11 DATA GROUP K: Stability and Accuracy Criteria--

Record 1--Maximum concentrations for all eight systems are required.

Record 2--Minimum concentrations for all eight systems are required.

2.4.2.12 DATA GROUP L: Intermediate Print Control--

No changes.

2.4.2.13 DATA GROUP M: Integration Control--

No changes.

2.4.2.14 DATA GROUP N: Print Tables--

Input is repeated 8 times, once for each system.

Record 1--Variable Names

EUTRWASP displays the following variables for ANAME(K):

System 1: Ammonia, flow, ambient segment temperature, preference factor.

System 2: Nitrate plus nitrate nitrogen, total nitrogen, total inorganic nitrogen, nitrogen limitation factor for phytoplankton growth.

System 3: Ortho-phosphate phosphorous, total phosphorus, nutrient limitation indicator, phosphorus limitation factor.

System 4: Phytoplankton chlorophyll, phytoplankton carbon, light limitation factor, nutrient limitation factor.

System 5: Carbonaceous BOD, ultimate BOD, sediment oxygen demand, five day BOD.

System 6: Dissolved oxygen, dissolved oxygen deficit, minimum diurnal DO value, maximum diurnal DO value.

System 7: Organic nitrogen, total organic nitrogen, reaeration rate constant, ambient phytoplankton growth rate.

System 8: Organic phosphorous, total organic phosphorous, inorganic nitrogen to phosphorous ratio, ambient light extinction coefficient.

2.4.2.15 DATA GROUP O: Time Plots--

No changes.

2.4.2.16 DATA GROUP P: Spatial Plots--

No changes.

2.4.3 EUTRWASP Data Group Tables

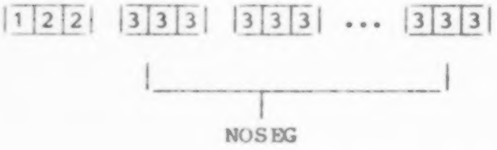
DATA GROUP G

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NOPAM	I5	1-10	No. of parameters required = 13.
	TITLE	5A4	61-80	"G: Environmental Parameters".
2	SCALP(1)	E10.3	1-10	Scale factor for DEPTH.
	SCALP(2)	E10.3	11-20	Not relevant.
	SCALP(3)	E10.3	21-30	Not relevant
	SCALP(4)	E10.3	31-40	Scale factor for VELSGM.
	SCALP(5)	E10.3	41-50	Scale factor for TMPSG.
	SCALP(6)	E10.3	51-60	Not relevant.
	SCALP(7)	E10.3	61-70	Scale factor for KESG.
	SCALP(8)	E10.3	71-80	Not relevant.
2	SCALP(9)	E10.3	1-10	Scale factor for EDIF.
	SCALP(10)	E10.3	11-20	Scale factor for SOD1D.
	SCALP(11)	E10.3	21-30	Scale factor for FPIPWC.
	SCALP(12)	E10.3	31-40	Scale factor for FNH4.
	SCALP(13)	E10.3	41-50	Scale factor for EPO4.
3	DEPTH	A5	1-5	Depth of segment, ft^2
	PARAM(ISEG,1)	F10.0	6-15	
	TYPEE	A5	16-20	Flag designating segment type.
	PARAM(ISEG,2)	F10.0	21-30	
	BOTSG	A5	31-35	Segment below current segment.
	PARAM(ISEG,3)	F10.0	36-45	
	VELSG	A5	46-50	Water velocity, ft/sec.
	PARAM(ISEG,4)	F10.0	51-60	
	TMPSG	A5	61-65	Temperature multiplier, °C.
	PARAM(ISEG,5)	F10.0	66-75	
	TMPFN	A5	1-5	Flag designating the time-
	PARAM(ISEG,6)	F10.0	6-15	variable temp. function.
	KESG	A5	16-20	Extinction coefficient
	PARAM(ISEG,7)	F10.0	21-30	multiplier, 1/ft.
	KEFN	A5	31-35	Flag designating the time
	PARAM(ISEG,8)	F10.0	36-45	variable extinction coefficient
	EDIF	A5	46-50	Dispersion coefficient for ex-
	PARAM(ISEG,9)	F10.0	51-60	change of dissolved chemical.

DATA GROUP G (Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
	SOD1D	A5	61-65	Sediment oxygen demand, g/m^2/day.
	PARAM(ISEG10)	F10.0	66-75	
3	FPIPW	A5	1-5	Spatially variable of inorganic PO4 sorbed to particulates, and subject to settling.
	PARAM(ISEG11)	F10.0	6-15	
	FNH4	A5	16-20	Average ammonium flux multiplier, mg/m^2/day.
	PARAM(ISEG12)	F10.0	21-30	
	FPO4	A5	31-35	Average phosphate flux multiplier, mg/m^2/day.
	PARAM(ISEG13)	F10.0	36-45	

ORGANIZATION OF RECORDS



DATA GROUP H

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NCONS	I5	1-10	No. of constants required = 48
	TITLE	5A4	61-80	"H: Chemical Constants".
2	K1C	A5	1-5	Saturated growth rate of phytoplankton, 1/day.
	CONST(1)	F10.0	6-15	
	K1T	A5	16-20	Temperature coefficient.
	CONST(2)	F10.0	21-30	
	LGHTSW	A5	31-35	Light formulation switch.
	CONST(3)	F10.0	36-45	
	PHIMX	A5	46-50	Maximum quantum yield constant, mgC/mole photons.
	CONST(4)	F10.0	51-60	
	XKC	A5	61-65	Chlorophyll extinction coefficient, m^2/mgchla
	CONST(5)	F10.0	66-75	
2	CCHL	A5	1-5	Carbon-to-chlorophyll ratio, mg carbn/mgchla.
	CONST(6)	F10.0	6-15	
	IS1	A5	16-20	Saturation light, intensity for phytoplankton, ly/day.
	CONST(7)	F10.0	21-30	
	KMNG1	A5	31-35	Nitrogen half saturation constant for phytoplankton growth, mg/N/L.
	CONST(8)	F10.0	36-45	
	KMPG1	A5	46-50	Phosphorous half-saturation constant for phytoplankton growth, mg PO_4-P/L.
	CONST(9)	F10.0	51-60	
	K1RC	A5	61-65	Endogenous respiration rate of phytoplankton at 20°C, 1/day.
	CONST(10)	F10.0	66-75	
2	K1RT	A5	1-5	Temperature coefficient for phytoplankton growth.
	CONST(11)	F10.0	6-15	
	K1D	A5	16-20	Non-predatory phytoplankton death rate, 1/day.
	CONST(12)	F10.0	21-30	
	KMPHYT	A5	31-35	Half-saturation constant for phytoplankton, mg-carbon/L.
	CONST(13)	F10.0	36-45	
	PCRB	A5	46-50	Phosphorous-to-carbon ratio in phytoplankton, mg PO_4-P/mg.
	CONST(14)	F10.0	51-60	
	NCRB	A5	61-65	Nitrogen-to-carbon ratio in phytoplankton, mg N/mg C.
	CONST(15)	F10.0	66-75	
2	OCRB	A5	1-5	Oxygen-to-carbon ratio in phytoplankton, mg O_2/mg C.
	CONST(16)	F10.0	6-15	
	NUTLIM	A5	16-20	Nutrient limitation option.
	CONST(17)	F10.0	21-30	
	DUMMY	A5	31-35	Leave blank.
	CONST(18)	F10.0	36-45	
	FSBOD	A5	46-50	Fraction of the carbonaceous biochemical oxygen demand that settles.
	CONST(19)	F10.0	51-60	
	FSDP	A5	61-65	Fraction of the total non-living organic phosphorus that settles.
	CONST(20)	F10.0	66-75	

DATA GROUP H
(Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
2	FSIP	A5	1-5	Spatially-constant fraction of inorganic phosphorus that settles.
	CONST(21)	F10.0	6-15	
	FSON	A5	16-20	Fraction of total non-living organic nitrogen that settles
	CONST(22)	F10.0	21-30	
	K58C	A5	31-35	Mineralization rate of dissolved organic phosphorus, 1/day.
	CONST(23)	F10.0	36-45	
	K58T	A5	46-50	Temperature coefficient for K58C.
	CONST(24)	F10.0	51-60	
	K1013C	A5	61-65	Mineralization rate of dissolved organic, nitrogen, 1/day.
	CONST(25)	F10.0	66-75	
2	K1013T	A5	1-5	Temperature coefficient for K1013C.
	CONST(26)	F10.0	6-15	
	K1320C	A5	16-20	Nitrification rate at 20°C, 1/day.
	CONST(27)	F10.0	21-30	
	K1320T	A5	31-35	Temperature coefficient for K1320C.
	CONST(28)	F10.0	36-45	
	K140C	A5	46-50	Denitrification rate at 20°C, 1/day.
	CONST(29)	F10.0	51-60	
	K140T	A5	61-65	Temperature coefficient for K140C.
	CONST(30)	F10.0	66-75	
2	KNIT	A5	1-5	Half-saturation constant for nitrification-oxygen limitation, mg O_2/L.
	CONST(31)	F10.0	6-15	
	KNO3	A5	16-20	Half-saturation constant for denitrification oxygen limitation, mgO_2/L.
	CONST(32)	F10.0	21-30	
	KDC	A5	31-35	BOD deoxygenation rate at 20°C, 1/day.
	CONST(33)	F10.0	36-45	
	KDT	A5	46-50	Temperature coefficient for carbonaceous deoxygenation in water column.
	CONST(34)	F10.0	51-60	
	SVPL1	A5	61-65	Settling velocity of phytoplankton, 1/day.
	CONST(35)	F10.0	66-75	
2	SVPP	A5	1-5	Settling velocity of particulate phosphorus, ft/day.
	CONST(36)	F10.0	6-15	
	SVPN	A5	16-20	Settling velocity of particulate organic nitrogen, ft/day
	CONST(37)	F10.0	21-30	
	SVBOD	A5	31-35	Settling velocity of particulate BOD fraction, ft/day.
	CONST(38)	F10.0	36-45	
	SEDVEL	A5	46-50	Sediment velocity, in/yr.
	CONST(39)	F10.0	51-60	
	SCOUR	A5	61-65	Mean scour velocity, in/yr.
	CONST(40)	F10.0	66-75	

DATA GROUP H
(Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
2	KPZDC CONST(41)	A5 F10.0	1-5 6-15	Decomposition rate constant for phytoplankton in the sediment of 20°C, 1/day.
	KPZDT CONST(42)	A5 F10.0	16-20 21-30	Temperature coefficient for decomposition of phytoplankton in sediment.
	KOPDC CONST(43)	A5 F10.0	31-35 36-45	Decomposition rate of organic phosphorus in sediment at 20°C, 1/day.
	KOPDT CONST(44)	A5 F10.0	46-50 51-60	Temperature coefficient for decomposition of organic phosphorus in the sediment.
	KONDC CONST(45)	A5 F10.0	61-65 66-75	Decompsoition rate constant for organic nitrogen in the sediment at 20°C, 1/day.
2	KONDT CONST(46)	A5 F10.0	1-5 6-15	Temperature coefficient for decomposition of organic nitrogen in the sediment.
	KDSC CONST(47)	A5 F10.0	16-20 21-30	Decomposition rate of carbonaceous BOD in the sediment at 20°C, 1/day.
	KDST CONST(48)	A5 F10.0	31-35 36-45	Temperature coefficient for carbonaceous deoxygenation in the sediment.
	KBOD CONST(49)	A5 F10.0	46-50 51-55	Half saturation constant for carbonaceous deoxygenation oxygen limitation.

ORGANIZATION OF RECORDS

1	2	2	2	2	2	2	2	2	2	2

DATA GROUP I

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NFUNC	I5	1-5	No. time functions required = 14
	TITLE	5A4	61-80	"I: Time Functions."
2	TEMP(1)	A5	1-5	Time variable temp. function.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	VALT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	VALT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	VALT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	VALT(K)	F10.0	.	K = NOBRK(I)
	T(K)	F10.0	.	
2	TEMP(2)	A5	1-5	Time-variable temp. function.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	TEMP(3)	A5	1-5	Time-variable temp. function.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	TEMP(4)	A5	1-5	Time-variable temp. function.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	ITOT	A5	1-5	Total daily solar radiation, ly.
	NOBRK	I5	6-10	Number breaks used.

DATA GROUP I
(Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	F	A5	1-5	Fraction of day light, day.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	WIND	A5	1-5	Wind velocity, ft/sec.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	KE(1)	A5	1-5	Time variable extinction coef. function.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	KE(2)	A5	1-5	Time variable extinction coef. function.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	N = NOBRK
2	KE(3)	A5	1-5	Time variable extinction coef. function.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 11

DATA GROUP I
(Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	KE(4)	A5	1-5	Time variable extinction coef.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	KE(5)	A5	1-5	Time variable extinction coef.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	TFNH4	A5	1-5	Normalized ammonium flux from bed.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK
2	TFPO4	A5	1-5	Normalized phosphate flux from bed.
	NOBRK	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	.	.	.	.
	.	.	.	.
	.	.	.	.
	VALT(K)	.	.	.
	T(K)	.	.	K = NOBRK

ORGANIZATION OF RECORDS

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2.4.4 Variable Definitions

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
AVDEPE	EU03K2	Average depth for a segment.	ft
AVVELE	EU03K2	Average velocity of a segment.	ft/sec
BOD5	EU03DU	5 Day biochemical oxygen demand.	mg/L
BOTSG(ISEG)	WASPB EU03SX EU03IN	The segment immediately below ISEG.	unit-less
CBOD	WASPB, EU03S5	Carbonaceous biochemical oxygen demand.	mg/L
CCHL*	EU03S4 EU03IN	Carbon to chlorophyll ratio (used only in Di Toro's light formulation) varies in time if Dick Smith's light formulation is used--constant is internally calculated.	mg carbon/ mg chla
CCHL1	EU03S4	Carbon to chlorophyll ratio that varies in time if Dick Smith's light formulation is used.	mg/ carbon/ mg chla
CFOREA	EU03K2	Fraction of surface area affected by wind-driven reaeration, set equal to 1.0.	ft^2/ ft^2
CN	EO03S4	Total inorganic nitrogen.	mg/L
CS	EU03S6 EU03DU	Dissolved oxygen saturation concentration.	mg/L
DELO2	EU03DU	Diurnal dissolved oxygen variation.	mg/L
DERIV	EU03S3 EU03S7 EU03S8	Intermediate kinetic derivative.	mg/L MCF/ day
DIF	EU03K2	Internal variable used to determine whether Churchill's or O'Connor-Dobbin's reaeration formula is used.	unit-less
DEATH	EU03S5	Phytoplankton death rate.	mg/L-day

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
DEPTH(ISEG)	WASPB	Depth of ISEG.	ft
DEPTHM	WASPB EU03S6	Depth of segment.	m
DODEF	EU03DU	The dissolved oxygen deficit.	mg/L
DOMAX	EU03DU	DO + DELO2/2 maximum diurnal DO.	mg/L
DOMIN	EU03DU	DO - DELO2/2 minimum diurnal DO.	mg/L
DPP	EU03S4 EU03S5 EU03S7 EU03S8	Phytoplankton death rate.	m/(1 day^{-1})
DO	WASPB EU03DU EU03S6 EU03S1	Dissolved oxygen concentration.	mg/L
DP1	EU03S4	Specific phytoplankton death rate constant (Respiration + Death).	day^{-1}
DTDAY	EU03S4	Time of day increment (expressed as decimal fraction) used in integrating Smith light formulation over day.	unitless
EDIF(ISEG)	EU03IN EU03SX	Dispersion coefficient for exchange of dissolved chemical between ISEG and IBOT; Converted to dispersion volume internally, million ft^3/day.	cm^2/day
EXCH	EU03SX	Dispersive volume exchanged between benthic and water column segments.	MCF/day
EXPRED	EU03K2	Depth exponent used reaeration calculations.	unitless
EXPREV	EU03K2	Velocity exponent used in reaeration calculations.	unitless
F*	EU03S4	Fraction of day that is daylight, input as time function.	days
FLOW	EU03DU	Flow.	MCF/day

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
FNH_4(ISEG)*	EU03IN EU03SX	Average ammonium-N flux multiplier for segment ISEG, input parameter for water column networks.	unitless
FLUX	EU03SX S1,S2,S3, S4,S5,S6, S7,S8	Rate at which a constituent settles to or exchanges with a lower segment.	mg/L
FP04(ISEG)*	EU03IN EU03SY	Average phosphate-P flux multiplier for segment ISEG input parameter for water column networks.	unitless
FPIPWC* (ISEG)	EU03S3	Spatially variable fraction of inorganic phosphorus that is sorbed to particulate and settles.	unitless
FSBOD*	EU0355	Fraction of the carbonaceous biochemical oxygen demand that settles.	unitless
FSIP*	EU03S3	Spatially-constant fraction of inorganic phosphorus that is sorbed to particulate and settles.	unitless
FSON*	EU03S7	Fraction of non-living organic nitrogen that settles.	unitless
FSOP*	EU03S8	Fraction of non-living organic phosphorus that settles.	unitless
GITMAX	EU03S4	Maximum specific phytoplankton growth rate.	$days^{-1}$
GITMX1	EU03S4	Maximum specific phytoplankton growth rate corrected for temperature.	$days^{-1}$
GIT1	EU03S4	Light limited specific phytoplankton growth rate.	day^{-1}
GPP	EU03S4 EU03S3	Light and nutrient limited phytoplankton growth rate.	mg/L/day
GP1	EU03S4 EU03S6 EU03S1 EU03S2	Light and nutrient limited specific phytoplankton growth rate.	day^{-1}

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
H	WASPB EUO3K2	Depth of segment being considered.	ft
IAV	WASPB EUO3S4	Average light intensity during daylight hours, converted to Ly/min in Smith formulation.	Ly/day
IBOT	EUO3SX	The segment immediately below ISEG.	unit-less
IDFREC	WASPB	PDP version set up as a record pointer.	unit-less
IKE	EUO3S4	The number of the time-variable extinction coefficient used for ISEG.	unit-less
IMAX	EUO3S4	Maximum light intensity during the day.	Ly/day
IS1*	EUO3S4	Saturating light intensity for phytoplankton (used only if using Di Toro light formulation).	Ly/day
ITO	WASPB	The segment immediately below ISEG.	unit-less
ITOT*	WASPB, EUO3S4	Total daily solar radiation, input as time function.	Ly
IO	EUO3S4	Light intensity at surface of segment; a sinusoidal function used in Smith formulation.	Ly/day
KA	EUO3S6	Reaeration rate constant at segment temperature.	day^{-1}
KBOD	EUO3S5	Half saturation constant for oxygen limitation of carbonaceous deoxygenation.	mg/L
KDC*	EUO3S5	Specific carbonaceous BOD deoxyenation rate at 20°C.	day^{-1}
KDSC*	EUO3S5	Specific decomposition rate of carbonaceous BOD in benthos at 20°C.	day^{-1}
KDST*	EUO3S5	Temperature coefficient for carbonaceous deoxygenation in benthos.	unit-less

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
KDT*	EU03S5	Temperature coefficient for carbonaceous deoxygenation in water column	unitless
KE(I)	WASPB	Light extinction coefficient, time function number I = 1-5.	ft^{-1}
KEFN(ISEG)	EU03S4	Light extinction time function chosen for ISEG.	unitless
KESG(ISEG)	EU03S4	Average light extinction multiplier for ISEG.	unitless
KESHD	EU03S4	Phytoplankton self-shading coefficient, used in Di Toro formulation.	ft^{-1}
KMNG1*	EU03S4	Nitrogen half saturation constant for phytoplankton growth, which also affects ammonia preference.	mg-N/L
KMPG1	EU03S4	Phosphorus half saturation constant for phytoplankton growth.	mg PO_4-P/L
KMPHYT*	EU03S4	Half saturation constant for phytoplankton effects on mineralization of organic phosphorus and nitrogen.	mg CRB/L
KNIT*	EU03S5	Half saturation constant for oxygen limitation of nitrification.	mg O_2/L
KNO3*	EU0352	Half saturation constant for denitrification oxygen limitation.	mgO_2/L
KONDC*	EU03S7	Decomposition rate constant for organic nitrogen in the benthos at 20°C.	day^{-1}
KONDT*	EU03S7	Temperature coefficient for decomposition of organic nitrogen in the benthos.	unitless
KOPDC*	EU03S8	Decomposition rate constant for organic phosphorus in the benthos at 20°C.	day^{-1}
KOPDT*	EU03S8	Temperature coefficient for decomposition of organic phosphorus in the benthos.	unitless
KOREA	EU03K2	Reaeration rate constant based on wind speed, surface area, and volume.	day^{-1}

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
KPZDC*	EU03S4	Specific decomposition rate of phytoplankton in the benthos at 20°C.	day^{-1}
KPZDT*	EU03S4	Temperature coefficient for decomposition of phytoplankton in the benthos.	unitless
K1C*	EU03S4	(Const). Maximum saturated growth rate of phytoplankton at 20°C.	day^{-1}
K1D*	EU03S4 EU03S5	(Const). Non-predatory phytoplankton death rate.	day^{-1}
K1RC*	EU03S4	Endogenous respiration rate for phytoplankton at 20°C.	unitless
K1RT*	EU03S4	Temperature coefficient for phytoplankton respiration	unitless
K1T*	EU03S4	(Const). Temperature coefficient for phytoplankton growth.	unitless
K1013C*	EU03S7	Mineralization rate constant for dissolved organic nitrogen.	day^{-1}
K1013T*	EU03S7	Temperature coefficient for mineralization of dissolved organic nitrogen.	unitless
K1320C*	EU03S1	Nitrification rate constant at 20°C.	day^{-1}
K1320T*	EU03S1	Temperature coefficient for nitrification.	unitless
K140C*	EU0352	Denitrification rate at 20°C.	day^{-1}
K140T*	EU0352	Temperature coefficient for K140C.	unitless
K20	EU03K2 EU03S6	Reaeration rate constant at 20°C.	day^{-1}
K58C*	EU03S8	Mineralization rate constant for dissolved organic phosphorous.	day^{-1}
K58T*	EU03S8	Temperature coefficient for mineralization of dissolved organic phosphorus.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
LGHTSW*	EU03S4	Light formulation switch: 0 = use Dick Smith's (USGS) formulation; 1 = use Di Toro et al. (1971) formulation.	unitless
LIMIT	EU03DU	Nutrient limitation indicator ("+" = nitrogen, "-" = phosphorus).	unitless
NCRB*	EU03S1, EU03S2, EU03S7	Nitrogen to carbon ratio in phytoplankton.	mg N/ mg CRB
NH3	WASPB, EU03S1, EU03S4, EU03DU	Segment ammonia concentration.	mg-N/L
NO3	WASPB, EU03DU	Segment nitrite and nitrate nitrogen concentration.	mg-N/L
NUTLIM*	EU03S4	Nutrient limitation option: 0 = minimum; 1 = multiplicative.	unitless
OCRB*	EU03S5	Oxygen to carbon ratio in phytoplankton.	mg-O_2/ mg CRB
ON	WASPB, EU03S7, EU03DU	Segment organic nitrogen concentration.	mg/L
OP	WASPB, EU03S8, EU03DU	Segment organic phosphorus concentration.	mg/L
OPO4	WASPB, EU03S3, EU03DU	Segment orthophosphate concentration.	mg/L
PCRB*	EU03S3, EU03S8	Phosphorus to carbon ratio in phytoplankton.	mg PO_4-p/mgCRB
PHIMX*	EU03S4	Maximum quantum yield constant (used with Smith formulation).	mg CRB/ mole photons
PHYT	WASPB, EU03S4, EU03IN, EU03S1,	Phytoplankton biomass as carbon.	mg/L

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
	EU03S2, EU03S6		
PI	EU03S4	Math function Pi.	
PNH3G1	EU03S4, EU03S1, EU03S2	Preference factor for ammonia over nitrate.	unitless
RATIO	EU03DU	Inorganic nitrogen to phosphorus ratio.	mg/mg
REAK	EUK03K2	Multiplier used in calculating reaeration rate.	unitless
RESP	EU03S4, EU03S6	Phytoplankton respiration rate.	mg/L/day
RLIGHT	EU03S4	Light limitation factor for phytoplankton growth.	unitless
RNUTR	EU03S4	Nutrient limitation factor for phytoplankton.	unitless
SA	EU03IN	Surface area of current segment.	million ft^2
SCOUR	EU03IN EU03S3 EU03S4 EU03S5 EU03S7 EU03S8	Mean scour velocity. NOTE: Gross deposition = scour + SEDVEL	in/yr
SDEPTH	EU03IN	Depth of surficial benthic sediment layer.	ft
SEDSEG	WASPB, EU03IN, EU03S3, EU03S4, EU03S5, EU03S6, EU03S7, EU03S8	Sediment segment indicator; .FALSE. = water column segment; .TRUE. = sediment segment.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
SEDVEL*	EU03IN, EU03S3, EU03S4, EU03S5, EU03S7, EU03S8	Sedimentation velocity converted internally, converted to ft/day internally.	in/yr
SKE	EU03S4	Total ambient light extinction coefficient.	ft^{-1}
SK1013	EU03S1, EU03S7	Rate at which organic nitrogen is mineralized to ammonia.	mg/(L-day)
SK13P1	EU03S1	Rate at which ammonia is taken up by phytoplankton.	mg/(L-day)
SK1314	EU03S1, EU03S2, EU03S6	Rate at which ammonia is nitrified to nitrate.	mg/(L-day)
SK14P1	EU03S2	Rate at which nitrate is taken up by phytoplankton.	mg/(L-day)
SK140D	EUO352 EUO355	Rate at which nitrate is reduced by denitrification	mg/(L-day)
SK180D	EUO355	Rate at which CBOD is reduced by denitrification.	mg/CL-day
SK180	EU03S5, EU03S6	Rate at which CBOD is oxidized.	mg/(L-day)
SK19P	EU03S6	Rate at which oxygen is consumed by phytoplankton respiration.	mg/(L-day)
SK19S	EU03S6	Rate at which oxygen is consumed by benthic sediments.	mg/(L-day)
SK1913	EU03S6	Rate at which oxygen is consumed by nitrification.	mg/(L-day)
SK1918	EU03S6	Rate at which oxygen is consumed by CBOD.	mg/(L-day)
SK58	EU03S8, EU03S3	Rate at which organic phosphorus is mineralized to phosphate.	mg/(L-day)

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
SK8P	EU03S3	Rate at which phosphate is taken up by phytoplankton.	mg/(L-day)
SOD	EU03DU	Sediment oxygen demand.	gDO/(m^2-day)
SOD1D(ISEG)	EU03DU, EU03S6	Sediment oxygen demand input for 1-D networks.	gDO/(m^2-day)
SR130N	EU03S1	Rate at which ammonia is mineralized from organic nitrogen.	mg/(L-day)
SR1413	EU03S2	Rate at which nitrate is nitrified from ammonia.	mg/(L-day)
SR18P	EU03S5	Rate at which CBOD is generated from phytoplankton death.	mg/(L-day)
SR19PA	EU03S6	Rate at which DO is produced by phytoplankton growth using CO_2 and NH_3.	mg/(L-day)
SR19PB	EU03S6	Rate at which DO is produced by phytoplankton growth using CO_2 and NO_3.	mg/(L-day)
SR190	EU03S6	Rate at which DO is added by reaeration.	mg/(L-day)
SR5P	EU03S8	Rate at which organic phosphorus is produced from phytoplankton respiration and death.	mg/(L-day)
SR80P	EU03S3	Rate at which phosphate is mineralized from organic phosphorus.	mg/(L-day)
STP	WASPB, EU03DU	Temperature of the segment being considered.	C°
STP20	EU03S1, EU03S2, EU03S3, EU03S4, EU03S5, EU03S6, EU03S7, EU03S8	Difference between segment temperature and 20°C.	°C
SUM	EU03S4	Temporary variable used in integrating Smith light formulation over day.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
SVBOD*	EU03S5	Settling velocity of particulate BOD fraction.	ft/day
SVPN*	EU03S7	Settling velocity of particulate organic nitrogen.	ft/day
SVPP*	EU03S3, EU03S8	Settling velocity of particulate phosphorus.	ft/day
SVP1*	EU03S4	Settling velocity of phytoplankton.	ft/day
SW16A	WASPB, EU03S4	Internal switch indicating the passage of a day, used to trigger Smith light integration.	unitless
TCHLA	EU03DU EU03S4	Phytoplankton chlorophylla concentration	mg/l
TCHLAX	EU03DU	Phytoplankton chlorophylla concentration.	ug/L
TEMP(I)	WASPB	Temperature time function No. I (I = 1-4) for segments indicated by TMPFN (ISEG).	°C
TFNH4	EU03SX	Normalized time function for ammonium flux from bed.	mg-N/(m^2-day)
TFPO4	EU03SX	Normalized time function for phosphate flux from bed.	mg-P/(m^2-day)
TIN	EU03DU	Total inorganic nitrogen concentration.	mg/L
TIP	EU03DU	Total inorganic phosphorus concentratin.	mg/L
TMPSG	WASPB	Average water temperature multiplier for ISEG.	unitless
TMPFN(ISEG)	WASPB	Temperature time function chosen for ISEG.	unitless
TN	EU03DU	Total nitrogen concentration.	mg/L
TON	EU03DU	Total organic nitrogen concentration.	mg/L
TOP	EU03DU	Total organic phosphorus concentration.	mg/L

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
TRANDP	EUO3K2	The transition depth used to determine which reaeration formula should be used for a given current velocity.	ft.
TYPEE(ISEG)	WASPB EUO3IN EUO3SX	Type of segment: 1 = surface water 2 = subsurface water 3 = surface bed	unit-less
T16A	WASPB	Elapsed fraction of day, set to 0 at end of each day, used to trigger SW16A.	unit-less
UBOD	EUO3DO	Ultimate (30 day) BOD.	mg/L
VEL	EUO3S3, EUO3S4, EUO3S5, EUO3S7, EUO3S8	Generalized settling velocity, used internally.	ft/day
VELSG(ISEG)	WASPB	Water velocity in ISEG	ft/sec
VELSGM	WASPB, EUO3K2	Water velocity in a segment.	ft/sec
VOL	WASPB, EUO3DU	Volume of current segment.	million ft^3
WIND*	WASPB	Time-varying wind velocity.	ft/sec
WINDF	EUO3K2	Windspeed factor influencing reaeration.	cm/hr
WINDSG	WASPB, EUO3K2	Time varying wind velocity.	ft/sec
XEMPRC	EUO3S4, EUO3S7, EUO3S8	Phytoplankton limitation factor for the mineralization of organic nitrogen and organic phosphorus.	unit-less
XEMP1	EUO3S4	Nitrogen limitation factor for phytoplankton.	unit-less
XEMP2	EUO3S4	Phosphorus limitation factor for phytoplankton.	unit-less
XKC*	EUO3S4	Chlorophyll extinction coefficient used with Smith light formulation.	$(mg\ chl\text{-}a/m^3)^{-1}/m$

2.5 THE TOXICS MODEL

2.5.1 Introduction

TOXIWASP requires the same input format as the basic WASP3 model. This format is explained in detail in Section 2.3. This section describes variables needed specifically for TOXIWASP. Elaborations on WASP3 occur only in Data Groups G, H, and I. Records or variables within a record that are not mentioned here remain the same as described in Section 2.3.

As mentioned in Table 19, the 2 systems for toxics modeling are chemical and sediment. In data groups E, F, J, N, and O, input will be repeated twice, once for each system.

2.5.2 TOXIWASP Data Group Descriptions

2.5.2.1 DATA GROUP A: Model Identification and System Bypass Option--

Record 1--Model Identification

NOSYS = 2 for TOXIWASP.

2.5.2.2 DATA GROUP B: Exchange Coefficients--

No changes.

2.5.2.3 DATA GROUP C: Volumes--

No changes.

2.5.2.4 DATA GROUP D: Flows--

No changes.

2.5.2.5 DATA GROUP E: Boundary Concentrations--

No changes. Input is repeated twice, once for each system.

2.5.2.6 DATA GROUP F: Waste Loads--

No changes. Input is repeated twice, once for each system.

2.5.2.7 DATA GROUP G: Environmental Parameters--

VARIABLES

Record 1--Number of Parameters

NOPAM = 18 for TOXIWASP.

TITLE = name of data group.

Record 2--Scale Factors for Parameters

SCALP(K) = scale factor for parameter K.

K = 1, NOPAM

Record 3--Segment Parameters

ANAME(K) = an optional one to five alpha-numeric character descriptive name for parameter PARAM(ISEG,K).

PARAM(ISEG,K) = the value of parameter ANAME(K) in segment ISEG.

K = 1, NOPAM

ISEG = 1, NOSEG

Listed below are the 18 parameters required by TOXIWASP. Enter these names and their respective values in place of ANAME(K) and PARAM(ISEG,K).

K	PARAM(ISEG,K)	ANAME(K)	Definition and Units
1	TEMPM(ISEG,1)	TEMSG	Average temperature for segment (degrees C).
2	DEPTHG(ISEG,2)	DEPTH	Depth of segment (feet).
3	VELOC(ISEG,3)	VELOC	Average velocity of water in segment (feet per second).
4	WINDG(ISEG,4)	WINDG	Average wind velocity 10 cm above the water surface (surface water segments only) (meters per second).
5	TYPEE(ISEG,5)	TYPEE	Flag designating segment type.
6	BACTOG(ISEG,6)	BACTO	Bacterial population density in segment (cells per milliliter (water) cells per 100 grams dry weight (bed)).

K	PARAM(ISEG,K)	ANAME(K)	Definition and Units
7	ACBACG(ISEG,7)	ACBAC	Proportion of bacterial population that actively degrades chemical (dimensionless ratio).
8	BIOMAS(ISEG,8)	BIOMS	Total actively sorbing biomass in segment (mg (dry weight) per liter (water) or grams (dry weight) per square meter (bed)).
9	BIOTMG(ISEG,9)	BIOTM	Biotemperature in segment (degrees C).
10	POHG(ISEG,10)	POHG	Hydroxide ion activity in segment (pOH units).
11	OXRADG(ISEG,11)	OXRAD	Molar concentration of environmental oxidants in segment (moles per liter).
12	OCS(ISEG,12)	OCS	Organic carbon content of sediments as fraction of dry weight (dimensionless).
13	PCTWA(ISEG,13)	PCTWA	Percent water in benthic sediments, expressed as fresh/dry weight; all values must be greater than or equal to 1 (dimensionless).
14	DSPSED(ISEG,14)	DSPSD	Fraction of sediment volume that mixes (dimensionless).
15	PHG(ISEG,15)	PHG	Hydrogen ion activity in segment (pH units).
16	WS(ISEG,16)	WS,WR, or QP	Spatially variable parameter denoting settling rate of suspended sediment in water column segments (types 1 and 2), erosion rate of surface bed sediment in surface bed segment (type 3), or percolation of pore water through subsurface bed segments (type 4) (meters per day (1, 2); cm per year (3); cubic feet per second (4)).
17	CMPETG(ISEG,17)	CMPET	Single-valued zenith light extinction coefficients (for water segments only) (per meter).
18	TOTKG(ISEG,18)	TOTKG	Total first order decay rates calculated externally. If equal to zero, the program evaluates all separate processes and calculates a combined total first order decay rate internally (per day).

ORGANIZATION OF RECORDS

Record 1 is input once in Data Group G, occupying one line. Record 2 has 18 entries occupying 24 lines with eight entries per line. Record 3 has 18 entries per segment. At five entries per line, four lines are used for each segment.

2.5.2.8 DATA GROUP H: Chemical Constants--

VARIABLES

Record 1--Number of Constants

NCONS = 66 for TOXIWASP.

TITLE = name of data group.

Record 2--Constants

ANAME(K) = an optional one to ive alpha-numeric character descriptive name for constant CONST(K).

CONST(K) = the value of constant ANAME(K).

K = 1, 66

Listed below are the 66 constants required for eutrophication. Enter these variable names and their values, respectively, for ANAME(K) and CONST(K).

K	CONST(K)	ANAME(K)	DEFINITION AND UNITS
1,2,3	EBHG(I,1)	EBHG1 EBHG2 EBHG3	Arrhenius activation energy of specific-base-catalyzed hydrolysis of the toxicant (kcal/gram mole).
4,5,6	ENHG(I,1)	ENHG1 ENHG2 ENHG3	Arrhenius activation energy of neutral hydrolysis of the toxicant (kcal/gram mole).
7,8,9	EAHG(I,1)	EAGH1 EAHG2 EAGH3	Arrhenius activation energy of specific-acid-catalyzed hydrolysis of toxicant (kcal/gram mole).
10,11,12	KAHG(I,1)	KAHG1 KAHG2 KAHG3	Second-order rate constants for specific-acid=catalyzed hydrolysis of chemical (per mole [H+] per hour).

K	CONST(K)	ANAME(K)	DEFINITION AND UNITS
13,14,15	KBHG(I,1)	KBHG1 KBHG2 KBHG3	Second-order rate constants for specific-base-catalyzed hydrolysis of chemical (per mole [OH-] per hour).
16,17,18	KNHG(I,1)	KNHG1 KNHG2 KNHG3	Rate constants for neutral hydrolysis of organic chemical (per hour).
19,20,21	EOXG(I,1)	EOXG1 EOXG2 EOXG3	Arrhenius activation energy of oxidative transformation of the chemical (kcal/gram mole).
22,23,24	KOXG(I,1)	KOXG1 KOXG2 KOXG3	Second-order rate constants for oxidative transformation of toxicant (liter per mole environmental oxidant per hour).
25,26,27	KBACWG(I,1)	KBCW1 KBCW2 KBCW3	Second-order rate constants for water column bacterial biolysis of the organic chemical (ml/cel-hour).
28,29,30	QTBAWG(I,1)	QTBW1 QTBW2 QTBW3	Q-10 values for bacterial transformation rate in the water column. Q-10 is the increase in the second-order rate constant resulting from a 10 degree C temperature increase (dimensionless).
31,32,33	KBACSG(I,1)	KBCS1 KBCS2 KBCS3	Second-order rate constants for benthic sediment bacterial biolysis of the organic (ml/cell-hour).
34,35,36	QTBASG(I,1)	QTBS1 QTBS2 QTBS3	Q-10 values for bacterial transformation of organic chemical in benthic sediments. The Q-10 is the increase in the second-order rate constant resulting from a 10 degree C temperature increase (dimensionless).
37	KOC	KOC	Organic carbon partition coefficient (l_w/kg organic carbon).
38	KOW	KOW	Octanol water partition coefficient (l_w/loct).
39	OCB	OCB	Organic carbon content of the compartment biomass as a fraction of dry weight (dimensionless).

K	CONST(K)	ANAME(K)	DEFINITION AND UNITS
40	DUMMY	DUMMY	Leave blank.
41	DUMMY	DUMMY	Leave blank.
42	DUMMY	DUMMY	Leave blank.
43	MWTG	MWTG	The molecular weight of the chemical (grams per mle).
44	HENRYG	HENRY	Henry's Law constant of the toxicant (Atmosphere-cubic meters per mole).
45	VAPRG	VAPRG	Vapor pressure of compound (torr).
46	KVOG	KVOG	Measured experimental value for (volatilization) liquid-phase transport resistance, expressed as a ratio to the reaeration rate (dimensionless).
47	SOLG	SOLG	Aqueous solubility of toxicant chemical species (mg/l_T).
48	ESOLG	ESOLG	Exponential term for describing solubility of the toxicant as a function of temperature (see SOLG) (kcal/gram mole).
49	EVPRG	EVPRG	Molar heat of vaporization for vapor pressure described as a function of temperature (see VAPRG) (kcal/gram mole).
50	EHENG	EHENG	Constant used to compute Henry's Law constants for volatilization as a function of environmental temperatures (TCELG). When EHENG is nonzero, the Henry's Law constant is computed as follows (kcal/gram mole): log HENRY = HENRYG-((1000.*EHENG)/(4.58*(TCELG+273.15)))
51	DUMMY	DUMMY	Leave blank.
52	DUMMY	DUMMY	Leave blank.
53	FAC	FAC	Multiplication factor for sedimentation time step. Recommended 0.1 (dimensionless).

K	CONST(K)	ANAME(K)	DEFINITION AND UNITS
54	KDPG	KDPG	A near-surface photolytic rate constant for the chemical (per hour).
55	RFLATG	RFLAT	Reference latitude for corresponding direct photolysis rate constant KDPG (degrees and decimal fraction (e.g., 40.72)).
56	CLOUDG	CLOUD	Average cloudiness in tenths of full sky cover (dimensionless, range of 0.0 to 10.0).
57	LATG	LATG	Geographic latitude of ecosystem (degrees and tenths (e.g., 37.2)).
58	DFACG	DFACG	Distribution function (ratio of optical path length to vertical depth) (dimensionless).
59,60,61	QUANTG(I,1)	QUAN1 QUAN2 QUAN3	Reaction quantum yield in photolytic transformation of chemical (dimensionless).
62	XJTR	XJTR	Reference segment for triggering event and frequency output. A value of zero will disable it (dimensionless).
63	CTRIG	CTRIG	Trigger concentration that defines a peak event (mgc/l_T).
64	DTOPT	DTOPT	Option to optimize time step, if set to 1 (dimensionless).
65	TDINT	TDINT	Time interval between recalculation of decay rates (days).
66	DUMMY	DUMMY	Leave blank.

ORGANIZATION OF RECORDS

Record 1 is entered once in Data Group H. Record 2 has 66 entries and uses 14 lines. Five entries (ANAME(K)-CONST(K) pairs) will fit per line.

2.5.2.9 DATA GROUP I: Kinetic Time Functions

VARIABLES

Record 1--Number of Time Functions

NFUNC = 5 for TOXIWASP

TITLE = name of data group.

Record 2--Time Function Descriptions

ANAME(K) = an optional one to five alpha-numeric character descriptive name for the time function K.

NOBRK(K) = number of breaks used to describe the time function K.

K = 1, 5

Listed below are the five time functions required by TOXIWASP. Enter the variable names for ANAME(K) in Record 2 and their respective values for VALT(K) and T(K) in Record 3.

K	ANAME(K)		VALT(K)
1	TEMPN	=	Normalized temperature (dimensionless)
2	WINDN	=	Normalized wind speed (dimensionless)
3	PHN	=	Normalized pH (dimensionless)
4	POHN	=	Normalized pOH (dimensionless)
5	LIGHTN	=	Normalized light intensity (dimensionless)

Record 3--Time Functions

VALT(K) = value of the function at time T(K).

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK).

K = 1, NOBRK

ORGANIZATION OF RECORDS

Record 1 is entered once in Data Group I. Records 2 and 3, as a set, are repeated 5 times. Within each set, Record 2 is input once and Record 3 uses an many 80-space lines as needed to input NOBRK entries. Four entries (four VALK(K)-T(K) pairs) will fit on each 80-space line.

2.5.2.10 DATA GROUP J: Initial Conditions--

No changes. Input is repeated twice, once for each system.

2.5.2.11 DATA GROUP K: Stability and Accuracy Criteria--

No changes.

2.5.2.12 DATA GROUP L: Intermediate Print Control--

No changes.

2.5.2.13 DATA GROUP M: Integration Control--

No changes.

2.5.2.14 DATA GROUP N: Print Tables

Input is repeated twice, once for each system

Display variables are listed in Table 21.

2.5.2.15 DATA GROUP O: Time Plots

Input is repeated twice, once for each system. No changes.

2.5.2.16 DATA GROUP P: Spatial Plots

No changes.

2.5.3 TOXIWASP Data Group Tables

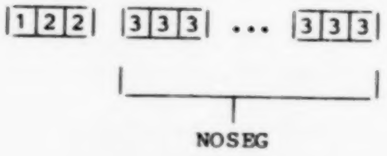
DATA GROUP G

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NOPAM	I5	1-10	No. of parameters required = 13.
	TITLE	5A4	61-80	"G: Environmental Parameters".
2	SCALP(1)	E10.3	1-10	Scale factor for TEMPM.
	SCALP(2)	E10.3	11-20	Scale factor for DEPTHG.
	SCALP(3)	E10.3	21-30	Scale factor for VELOC
	SCALP(4)	E10.3	31-40	Scale factor for WINDG.
	SCALP(5)	E10.3	41-50	Not relevant.
	SCALP(6)	E10.3	51-60	Scale factor for BACTOG
	SCALP(7)	E10.3	61-70	Scale factor for ACBACG.
	SCALP(8)	E10.3	71-80	Scale factor for BIOMAS.
2	SCALP(9)	E10.3	1-10	Scale factor for BIOTMG.
	SCALP(10)	E10.3	11-20	Scale factor for POHGD.
	SCALP(11)	E10.3	21-30	Scale factor for OXRADG.
	SCALP(12)	E10.3	31-40	Scale factor for OCS.
	SCALP(13)	E10.3	41-50	Scale factor for PCTWA.
	SCALP(14)	E10.3	51-60	Scale factor for DSPSED.
	SCALP(15)	E10.3	61-70	Scale factor for PHG.
	SCALP(16)	E10.3	71-80	Scale factor for WS.
	SCALP(17)	E10.3	1-10	Scale factor for CMPETG.
	SCALP(18)	E10.3	11-20	Scale factor for TOTKG.
3	TEMSG	A5	1-5	Average temperature, °C.
	PARAM(ISEG,1)	F10.0	6-15	
	DEPTH	A5	16-20	Depth, ft.
	PARAM(ISEG,2)	F10.0	21-30	
	VELOC	A5	31-35	Average velocity, ft/sec.
	PARAM(ISEG,3)	F10.0	36-45	
	WINDG	A5	46-50	Average wind velocity, m/sec.
	PARAM(ISEG,4)	F10.0	51-60	
	TYPEE	A5	61-65	Segment type.
	PARAM(ISEG,5)	F10.0	66-75	
3	BACTO	A5	1-5	Bacterial population, cells/mL
	PARAM(ISEG,6)	F10.0	6-15	
	ACBAC	A5	16-20	Active bacterial fraction.
	PARAM(ISEG,7)	F10.0	21-30	
	BIOMS	A5	31-35	Total actively sorbing biomass, mg/L
	PARAM(ISEG,8)	F10.0	36-45	
	BIOTM	A5	46-50	Biotemperature, °C.
	PARAM(ISEG,9)	F10.0	51-60	
	POHG	A5	61-65	pOH.
	PARAM(ISEG10)	F10.0	66-75	

DATA GROUP G (Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
	OXRAD	A5	1-5	Concentration of oxidants,
	PARAM(ISEG11)	F10.0	6-15	moles/L
	OCS	A5	16-20	Organic carbon fraction of
	PARAM(ISEG12)	F10.0	21-30	sediments.
	PCTWA	A5	31-35	Percent water in benthic
	PARAM(ISEG13)	F10.0	36-45	sediments.
	DSPSD	A5	46-50	Fraction of sediment volume
	PARAM(ISEG14)	F10.0	51-60	that mixes.
	PHG	A5	61-65	pH.
	PARAM(ISEG15)	F10.0	66-75	
3	WS	A5	1-5	Settling, deposition, scour, or
	PARAM(ISEG16)	F10.0	6-15	plore water flow.
	CMPET	A5	16-10	Light extinction coefficient,
	PARAM(ISEG17)	F10.0	21-30	1/m.
	TOTKG	A5	31-35	Total first order decay rates
	PARAM(ISEG18)	F10.0	36-45	calculated externally, 1/day.

ORGANIZATION OF RECORDS



DATA GROUP H

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NCONS	I5	1-10	No. of constants required = 66
	TITLE	5A4	61-80	"H: Chemical Constants".
2	EBHG1 CONST(1)	A5 F10.0	1-5 6-15	Arrhenius activation energy of base hydrolysis, Kcal/gram-mole.
	EBHG2 CONST(2)	A5 F10.0	16-20 21-30	Arrhenius activation energy of base hydrolysis, Kcal/gram-mole.
	EBHG3 CONST(3)	A5 F10.0	31-35 36-45	Arrhenius activation energy of base hydrolysis, Kcal/gram-mole.
	ENHG1 CONST(4)	A5 F10.0	46-50 51-60	Arrhenius activation energy of neutral hydrolysis, Kcal/gram-mole.
	ENHG2 CONST(5)	A5 F10.0	61-65 66-75	Arrhenius activation energy of neutral hydrolysis, Kcal/gram-mole.
2	ENHG3 CONST(6)	A5 F10.0	1-5 6-15	Arrhenius activation energy of neutral hydrolysis, Kcal/gram-mole.
	EAHG1 CONST(7)	A5 F10.0	16-20 21-30	Arrhenius activation energy of acid-hydrolysis, Kcal/gram-mole.
	EAHG2 CONST(8)	A5 F10.0	31-35 36-45	Arrhenius activation energy of acid-hydrolysis, Kcal/gram-mole.
	EAHG3 CONST(9)	A5 F10.0	46-50 51-60	Arrhenius activation energy of acid-hydrolysis, Kcal/gram-mole.
	KAHG1 CONST(10)	A5 F10.0	61-65 66-75	Second-order rate constants for acid-catalyzed hydrolysis, L/mole/hr.
2	KAHG2 CONST(11)	A5 F10.0	1-5 6-15	Second-order rate constants for acid-catalyzed hydrolysis, L/mole/hr.
	KAHG3 CONST(12)	A5 F10.0	16-20 21-30	Second-order rate constants for acid-catalyzed hydrolysis, L/mole/hr.
	KBHG1 CONST(13)	A5 F10.0	31-35 36-45	Second-order rate constants for base catalyzed hydrolysis, L/mole/hr.
	KBHG2 CONST(14)	A5 F10.0	46-50 51-60	Second-order rate constants for base catalyzed hydrolysis, L/mole/hr.
	KBHG3 CONST(15)	A5 F10.0	61-65 66-75	Second-order rate constants for base catalyzed hydrolysis, L/mole/hr.

DATA GROUP H (Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
2	KNHG1	A5	1-5	Rate constants for neutral hydrolysis, 1/hr.
	CONST(16)	F10.0	6-15	
	KNHG2	A5	16-20	Rate constants for neutral hydrolysis, 1/hr.
	CONST(17)	F10.0	21-30	
	KNGH3	A5	31-35	Rate constants for neutral hydrolysis, 1/hr.
	CONST(18)	F10.0	36-45	
	EOXG1	A5	46-50	Arrhenius activation energy of oxidation, Kcal/gram-mole.
	CONST(19)	F10.0	51-60	
	EOXG2	A5	61-65	Arrhenius activation energy of oxidation, Kcal/gram-mole.
	CONST(20)	F10.0	66-75	
2	EOXG3	A5	1-5	Arrhenius activation energy of oxidation, Kcal/gram-mole.
	CONST(21)	F10.0	6-15	
	KOXG1	A5	16-20	Second-order rate constants for oxidation, L/mole oxidant/hr.
	CONST(22)	F10.0	21-30	
	KOXG2	A5	31-35	Second-order rate constants for oxidation, L/mole oxidant/hr.
	CONST(23)	F10.0	36-45	
	KOXG3	A5	46-50	Second-order rate constants for oxidation, L/mole oxidant/hr.
	CONST(24)	F10.0	51-60	
	KBCW1	A5	61-65	Second-order rate constants for water column biodegradation, mL/cell/hr.
	CONST(25)	F10.0	66-75	
2	KBCW2	A5	1-5	Second-order rate constants for water column biodegradation, mL/cell/hr.
	CONST(26)	F10.0	6-15	
	KBCW3	A5	16-20	Second-order rate constants for water column biodegradation, mL/cell/hr.
	CONST(27)	F10.0	21-30	
	QTBW1	A5	31-35	Q-10 values for water column biodegradation rate.
	CONST(28)	F10.0	36-45	
	QTBW2	A5	46-50	Q-10 values for water column biodegradation rate.
	CONST(29)	F10.0	51-60	
	QTBW3	A5	61-65	Q-10 values for water column biodegradation rate.
	CONST(30)	F10.0	66-75	
2	KBCS1	A5	1-5	Second-order rate constants for benthic biodegradation, mL/cell/hr.
	CONST(31)	F10.0	6-15	
	KBCS2	A5	16-20	Second-order rate constants for benthic biodegradation, mL/cell/hr.
	CONST(32)	F10.0	21-30	
	KBCS3	A5	31-35	Second-order rate constants for benthic biodegradation, mL/cell/hr.
	CONST(33)	F10.0	36-45	

DATA GROUP H (Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
	QTBS1	A5	46-50	Q-10 values for benthic biodegradation rate.
	CONST(34)	F10.0	51-60	
	QTBS2	A5	61-65	Q-10 values for benthic biodegradation rate.
	CONST(35)	F10.0	66-75	
2	QTBS3	A5	1-5	Q-10 values for benthic biodegradation rate.
	CONST(36)	F10.0	6-15	
	KOC	A5	16-20	Organic carbon partition coefficient, L_w/kg organic carbon
	CONST(37)	F10.0	21-30	
	KOW	A5	31-35	Octanol water partition coefficient, L_w/L_{oct}.
	CONST(38)	F10.0	36-45	
	OCB	A5	46-50	Organic carbon fraction of biomass.
	CONST(39)	F10.0	51-60	
	DUMMY	A5	61-65	
	CONST(40)	F10.0	66-75	Leave blank.
2	DUMMY	A5	1-5	
	CONST(41)	F10.0	6-15	Leave blank.
	DUMMY	A5	16-20	
	CONST(42)	F10.0	21-30	Leave blank.
	MWTG	A5	31-35	The molecular weight of the chemical, g/mole.
	CONST(43)	F10.0	36-45	
	HENRY	A5	46-50	Henry's Law constant of the toxicant, atmosphere-m^3/mole.
	CONST(44)	F10.0	51-60	
	VAPRG	A5	61-65	Vapor pressure of compound, torr.
	CONST(45)	F10.0	66-75	
2	KVOG	A5	1-5	Measured ratio - volatilization to reaeration.
	CONST(46)	F10.0	6-15	
	SOLG	A5	16-20	Aqueous solubility, mg/L
	CONST(47)	F10.0	21-30	
	ESOLG	A5	31-35	Solubility temperature correction, Kcal/mole.
	CONST(48)	F10.0	36-45	
	EVPRG	A5	46-50	Molar heat of vaporization, Kcal/gram mole.
	CONST(49)	F10.0	51-60	
	EHENG	A5	61-65	Constant used to compute Henry's Law constants, Kcal/gram mole.
	CONST(50)	F10.0	66-75	
2	DUMMY	A5	1-5	
	CONST(51)	F10.0	6-15	Leave blank.
	DUMMY	A5	16-20	
	CONST(52)	F10.0	21-30	Leave blank.
	FAC	A5	31-35	Multiplication factor for sedimentation time step.
	CONST(53)	F10.0	36-45	
	KDPG	A5	46-50	Reference photolytic rate constant, 1/hr.
	CONST(54)	F10.0	51-60	

DATA GROUP H (Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
	RFLAT	A5	61-65	Reference latitude for photolysis rate constant KDPG, degrees.
	CONST(55)	F10.0	66-75	
2	CLOUD	A5	1-5	Average cloudiness, in tenths of full sky cover.
	CONST(56)	F10.0	6-15	
	LATG	A5	16-20	Geographic latitude of ecosystem, degrees.
	CONST(57)	F10.0	21-30	
	DFACG	A5	31-35	Distribution function for light.
	CONST(58)	F10.0	36-45	
	QUAN1	A5	46-50	Photolytic reaction yield for dissolved, sorbed, and biosorbed phases.
	CONST(59)	F10.0	51-60	
	QUAN2	A5	61-65	Photolytic reaction yield for dissolved, sorbed, and biosorbed phases.
	CONST(60)	F10.0	66-75	
2	QUAN3	A5	1-5	Photolytic reaction yield for dissolved, sorbed, and biosorbed phases.
	CONST(61)	F10.0	6-15	
	XJTR	A5	16-20	Reference segment for triggering event and frequency out put.
	CONST(62)	F10.0	21-30	
	CTRIG	A5	31-35	Trigger concentration that defines a peak event, mgc/L_T.
	CONST(63)	F10.0	36-45	
	DTOPT	A5	46-50	Option to optimize time step, if set to 1.
	CONST(64)	F10.0	51-60	
	TDINT	A5	61-65	Time interval between recalculation of decay rates, days.
	CONST(65)	F10.0	66-75	
2	DUMMY	A5	1-5	Leave blank.
	CONST(66)	F10.0	6-15	

ORGANIZATION OF RECORDS:

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DATA GROUP I

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
1	NFUNC	I5	1-5	No. time functions required = 5.
	TITLE	5A4	61-80	"I: Time Functions".
2	TEMPN	A5	1-5	Normalized temperature.
	NOBRK(I)	I5	6-10	Number breaks used.
	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	VALT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	VALT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	VALT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
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	.	.	.	.
	VALT(K)	F10.0	.	K = NOBRK(I)
	T(K)	F10.0	.	
2	WINDN	A5	1-5	Normalized wind speed.
	NOBRK(I)	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	VALT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	VALT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	VALT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
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	.	.	.	.
	VALT(K)	F10.0	.	K = NOBRK(I)
	T(K)	F10.0	.	
2	PHN	A5	1-5	Normalized pH.
	NOBRK)I)	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	VALT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	VALT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	VALT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
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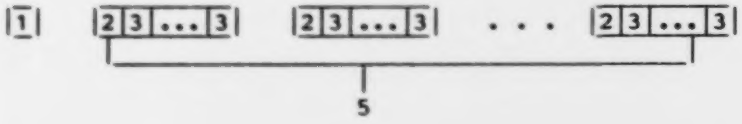
	.	.	.	.
	VALT(K)	F10.0	.	K = NOBRK(I)
	T(K)	F10.0	.	
2	POHN	A5	1-5	Normalized POH.
	NOBRK(I)	I5	6-10	Number breaks used.

DATA GROUP I (Continued)

RECORD	VARIABLE	FORMAT	COLUMN	SHORT DEFINITION
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1
	VALT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	VALT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	VALT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	VALT(K)	F10.0	.	K = NOBRK(I)
	T(K)	F10.0	.	
2	LIGHTN	A5	1-5	Normalized light intensity.
	NOBRK(I)	I5	6-10	Number breaks used.
3	VALT(K)	F10.0	1-10	Value of time functions.
	T(K)	F10.0	11-20	Time in days; K = 1.
	VALT(K)	F10.0	21-30	K = 2
	T(K)	F10.0	31-40	
	VALT(K)	F10.0	41-50	K = 3
	T(K)	F10.0	51-60	
	VALT(K)	F10.0	61-70	K = 4
	T(K)	F10.0	71-80	
	.	.	.	.
	.	.	.	.
	VALT(K)	F10.0	.	K = NOBRK(I)
	T(K)	F10.0	.	

ORGANIZATION OF RECORDS



2.5.4 TOXIWASP Variable Definitions

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
A(J)	MAIN	Cross sectional area between exchanging sediment and water compartments, input in subroutine WASP2.	ft^2
ACBACG(J)	TOXIWASPB TOXINIT TOXIFORD	Proportion of bacterial population that actively degrades toxicant. If the biolysis rate constants are not based on natural mixed bacterial populations, the total bacterial populations (BACTOG) given for each compartment can be modified via ACBACG to give the size of the population that is actively degrading the toxicant (nominal range: 0.0 - 1.0).	dimensionless ratio
ACBACL	TOXIFORD	Active bacterial population for segment being considered. Equal to BACTOG(J), Water column compartments: Benthic compartments:	cells/ml cells/ml pore water
ALPHA(I)	TOXIWASPB TOXIFORD TOXIDUMP TOXISETL TOXISEDW	The values of ALPHA are distribution coefficients (fraction of total concentration of toxicant (Y) present as a particular species/form configuration of the molecule) for each ecosystem compartment. ALPHA vector represents the plartitioning of each species among three physical forms (dissolved, sediment-sorbed, biosorbed). ALPHAs are calculated internally from the parameters, constants, and state variables describing the segment, including the predicted concentration, the sediment, the bimass, the octonol-water partition coefficient, etc. In the output these ALPHAs are designated by DISSF, SEDF and BIOLF. ALPHA(1) Fraction of toxicant present as the neutral molecule (SH2) dissolved in the water phase of the compartment.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
		ALPHA(2) Fraction present as neutral molecule sorbed with sediment phase of compartment. ALPHA(3) Fraction present as neutral molecule sorbed with compartment biomass.	
ALPH1M	TOXIWASPB TOXISEDW	Fraction of chemical sorbed onto sediment phase of the segment immediately above the bed. Equal to ALPHA(2) for that segment. Transferred to subroutine TOXISEDW for calculation of bed-water column mixing of chemical.	unitless
ALPH2M	TOXIWASPB TOXISEDW	Fraction of chemical sorbed onto sediment phase of the segment immediately above the bed. Equal to ALPHA(2) for that segment. Transferred to subroutine TOXISEDW for calculation of bed-water column mixing of chemical.	unitless
BACTOG(J)	TOXIWASPB TOXINIT TOXIFORD	Bacterial population density in each water column compartment. Benthic compartments: cells per 100 grams dry weight of sediment. Internally, BACTOG(J) is multiplied by ACBACG(J) to give active population density. For the sediment, BACTOG is converted to cells per milliliter pore water. The conversion used is: BACTOG(J) = BACTOG(J) * SED/FRW(1E08) where: $\text{BACTOG} = \frac{\text{cells}}{100\text{ g}} = \frac{\text{cells}}{100 * 1000\text{ mgs}}$ $\text{FRW} = \frac{l_w}{l_T} = \frac{ml_w}{l_T} * 1000$ $\text{SED(mg/ml)} = (1/1000)\text{SED}(\text{mg}/l_T)/\text{FRW}$	cells/ml

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
BETA	TOXIVOLT	Same as ALPHA(1) for water compartments that intersect surface.	unitless
BIOFAC	TOXIWASPB	Intermediate variable for determining fraction of chemical sorbed onto biological phase of a segment.	unitless
BIOMAS(J)	TOXIWASPB TOXINIT TOXIFORD	Total actively sorbing biomass in each ecosystem compartment. This parameter is used in computation of sorption of the toxicant on plant/animal material in the ecosystem compartments. The parameter is interpreted differently for the water column versus the benthic compartments. For a water column compartment, total biomass must be expressed as milligrams (dry weight) per liter of water in the compartment, and it includes all biomass subject to biosorptive exchange with that water. In the case of benthic compartments, BIOMAS is the total biomass of the benthic infauna and other components in grams (dry weight) per square meter of bottom. Note that in this simplification from EXAMS, movable biomass (e.g., plankton) is not distinguished from stationary biomass (e.g., roots). This is a potential source of error in systems having high biotic content. Water column compartments: mg (dry weight) per liter Benthic compartments: grams (dry weight) per square meter.	mg/L or g/m^2
BIOLKL	TOXIWASPB TOXIFORD TOXIDUMP	Total pseudo-first-order degradation rate constant (per hour) for bacterial biolysis.	hr^{-1}

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
BIOTMG(J)	TOXIWASPB TOXIFORD	Biotemperature in each exosystem compartment, i.e., temperature to be used in conjunction with Q-10 expressions for biolysis rate constants. This parameter is separated from the physical temperature input data (TCELG) in order that the input data can reflect Q-10 averaging of an observed temperature time-series.	°C
BMASS(J)	TOXIWASPB TOXIFORD TOXISETL	Mass of chemical lost from the network during the simulation. Chemical can be lost by volatilization through a surface water segment or burial through a bottom bed segment.	kg
BOTLIT	TOXIPHOT TOXINIT	Light level at bottom of compartment.	unitless
BURY	TOXISETL	Net burial or erosion rate of top benthic segment. Equal to the time variable depth of sediment settling in from the overlying water column minus the time-constant depth of sediment eroding. Both the settling and erosion rates are entered through the spatially-variable parameter WS (J).	m/yr
BVOLO(J)	TOXIWASPB TOXIFORD TOXISETL	Volume of the surface bed segment at time 0. The volume of the surface bed segment is reset to BVOLO during the compaction cycle.	million ft^3
CBB	TOXIWASPB TOXIDUMP	Concentration of chemical sorbed onto biological phase of bed segment JSTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	mg/g
CBW	TOXIWASPB TOXIDUMP	Concentration of chemical sorbed onto biological phase of water segment JTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	ug/g

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
CSB	TOXIWASPB TOXIDUMP	Concentration of chemical sorbed onto sediment phase of water segment JTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	mgc/kgs
CSW	TOXIWASPB TOXIDUMP	Concentration of chemical sorbed onto sediment phase of water segment JTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	mgc/kgs
CTB	TOXIWASPB TOXIDUMP	Total concentration of chemical in bed segment JSTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	mgc/L_T
CTW	TOXIWASPB TOXIDUMP	Total concentration of chemical in water segment JTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	mgc/L_T
C1B	TOXIWASPB TOXIDUMP	Concentration of chemical dissolved in water phase of bed segment JSTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	mgc/L_W
C1W	TOXIWASPB TOXIDUMP	Concentration of chemical dissolved in water phase at water segment JTR. Values transferred to TOXIDU every 3 hours for saving on the statistical file.	mgc/L_W
CHEM	TOXIWASPB TOXISETL TOXISEDW	Chemical concentration in segment, equivalent to C(J,1).	mg/L_T
CHEM1	TOXIDUMP	Chemical dissolved in water phase of current segment.	mgc/L_T
CHEM2	TOXIDUMP	Chemical sorbed onto sediment phase in current segment.	mgc/L_T
CHEM3	TOXIDUMP	Chemical sorbed onto biological phase in current segment.	mgc/L_T

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
CHEMB	TOXIDUMP	Chemical sorbed onto biological phase in current segment.	ugc/ $g_{biomass}$
CHEMS	TOXIDUMP	Chemical sorbed onto sediment phase in current segment.	mgc/kgs
CHEMW	TOXIDUMP	Chemical dissolved in water phase of current segment.	mgc/L_w
CHEM1S	TOXISEDW	Chemical concentration dissolved in pore water in bed segment.	mgc/L_w
CHEM2S	TOXISEDW	Chemical concentration sorbed on sediment in bed segment.	mgc/L_T
CHEMSS	TOXISEDW	Chemical concentration sorbed on sediment in bed segment.	mgc/kgs
CHEM1W	TOXISEDW	Chemical concentration dissolved in water segment above bed segment.	mgc/L_T
CHEM2W	TOXISEDW	Chemical concentration sorbed on sediment in water segment above bed segment.	mgc/L_T
CHEMSW	TOXISEDW	Chemical concentration on sorbed sediment in water segment above bed segment.	mgc/kgs
CLOUDG	TOXIWASP TOXIFORD TOXIPHOT	Average cloudiness in tenths of full sky cover (range of 0.0 to 10.0).	unitless
CMAX(9)	TOXIWASPB TOXINIT	The concentration of a 10^{-5} molar solution of chemical, or half the chemical solubility, whichever is less. CMAX(9) is used to abort the simulation whenever dissolved chemical concentration rises above this limit. This prevents violation of the model's first-order kinetics assumption. This check is activated only when CMAX(1) is set to 0.	mgc/L_w
CMAX(10)	TOXINIT	Half the chemical solubility.	mgc/L_w

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
CMPETG(J)	TOXIWASPB TOXIPHOT	Single-valued zenith light extinction coefficients for water columns, dummy variable for benthic compartments.	m^{-1}
COND	TOXIVOLT	Inverse of addition of series resistances of gas and liquid interfaces.	m/hr^{-1}
CTRIG	TOXIWASPB TOXINIT TOXIDUMP	Trigger concentration that defines a peak event. When the chemical concentration in segment JTR rises above CTRIG, a peak event is flagged. Concentrations for all segments are printed out every 3 hours until the concentration falls below CTRIG and the event ends. This option is designed to catch high transient concentrations that would be missed by the regular WASP dumps. If less frequent peak printout is desired, statement 68 in TOXIDUMP can be changed from PNEXT = 3.0 to, say PNEXT = 8.0. This would cause printouts every 8 hours during peak events. A trigger concentration of 0 will disable event printouts.	mgc/L_T
DELT	TOXIWASPB	Intermediate value of simulation time step used for maximizing time step to minimize numerical dispersion and simulation cost. Ranges between 0.01 and 0.50 days.	day
DENOM	TOXIWASPB	Intermediate variable for calculating fractions of chemical dissolved, sorbed onto sediment, and sorbed onto biomass.	unitless
DEPTH	TOXIWASPB TOXISETL	Depth of segment being considered.	ft
DEPTHG(J)	TOXIWASPB TOXIFORD TOXINIT TOXIVOLT TOXIPHOT TOXISETL	Depths of segments.	ft

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
DEPTHM	TOXIWASPB TOXIPHOT TOXISETL	Depth of segment being considered.	m
DFACG	TOXIWASPB TOXIPHOT	Distribution function (ratio of optical path length to vertical depth).	unitless
DISP	TOXISEDW	Volumetric dispersion between a bed and an overlying water segment, or between two vertically adjacent bed segments. DISP is brought from WASP2 using BR(I), and is corrected internally for its resulting mixed units.	MCF/sec $.cm^2/mi^2$
DISPV(J)	TOXIWASPB TOXISEDW	Dispersive exchange volumes between sediment and water compartments. Water-water exchanges are calculated in WASP2. Sediment-water exchanges are calculated in TOXISEDW using characteristic lengths, areas, and dispersion from WASP2, along with porosity and other factors from TOXISEDW.	million ft^3/day
DSPSED(J)	TOXIWASPB TOXISEDW	Fraction of sediment that mixes. 1.0 is equivalent to full bed sediment dispersion, 0.0 is equal to pore water diffusion only.	unitless
DTOPT	TOXIWASPB	Option to optimize time step. If set to 1, program computes maximum time that preserves numerical stability throughout network. Both flow volumes and dispersive exchange volumes are kept less than or equal to segment volumes. Time step can vary between 0.01 days and 0.5 days.	
E(J)		Sediment-water dispersion coefficient input in WASP2. E is a composite of direct sorption to the sediment surface, mixing of the sediments by benthic animals, stirring by demersal fishes, etc.	cm^3/sec
EAHG(I,1)	TOXIFORD	Arrhenius activation energy of specific-acid-catalyzed hydrolysis of the toxicant.	kcal/ gram mole

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
EBHG(I,1)	TOXIFORD	Arrhenius activation energy of specific-base-catalyzed hydrolysis of the toxicant.	kcal/ gram mole
EHENG	TOXIVOLT	Constant used to compute Henry's Law constants for volatilization as a function of environmental temperatures (TCELG). When EHENG is non-zero, the Henry's Law constant is computed as follows: log HENRY = HENRYG-((1000.*EHENG)/ (4.58*(TCELG+273.15)))	kcal/ gram mole
ENHG(I,1)	TOXIFORD	Arrhenius activation energy of neutral hydrolysis of the toxicant.	kcal/ gram mole
EOXG(I,1)	TOXIFORD	Arrhenius activation energy of oxidative transformation of the toxicant.	kcal/ gram mole
ESOLG	TOXIVOLT	Exponential term for describing solubility of the toxicant as a function of temperature (see SOLG).	kcal/ gram mole
EVPRG	TOXIVOLT	Molar heat of vaporization for vapor pressure described as a function of temperature (See VAPRG).	kcal/ gram mole
EXDO	TOXISEDW	Chemical sorption rate from lower water column segment to top bed segment.	MCF/day .mgc/L_T
EXUP	TOXISEDW	Chemical desorption rate from upper bed segment to lower water column segment.	MCF/day .mgc/L_T
FAC	TOXINIT	Multiplication factor for sedimentation time step. Set FAC to 1.0 to eliminate numerical dispersion in the bed. For smoother output with some numerical dispersion, set FAC to 0.1.	unitless
FACTOR	TOXIPHOT	Latitude correction factor by which the photolysis rate is adjusted from the rate at the reference latitude.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
FRW(J)	TOXIWASPB TOXINIT TOXISETL TOXISEDW	Porosity, or water fraction in sediment on a volumetric basis. Calculated from the parameter PCTWA(J).	L_w/L_T
FVOL	TOXISETL	The fractional volume of the surface bed segment that is to be compacted into the volume of the second bed segment during the compaction cycle. The difference between FVOL and the volume of the second bed segment is SVOL, the pore water squeezed out.	million ft^3
HENRYG	TOXIFORD TOXIVOLT	Henry's Law constant of the toxicant. If parameter EHENG is non-zero, HENRYG is used as the pre-exponential factor in computing the Henry's Law constant as a function of environmental temperature (TCELG).	m^3/mole
HENRYL	TOXIVOLT	Local value of HENRYG. If HENRYG is zero, model will calculate value.	m^3/mole
HPLUS	TOXIFORD	Intermediate calculation in obtaining temporally averaged concentration of hydronium ions. HPLUS = 10**(=PHG)	
HYDRKL	TOXIFORD TOXIDUMP	Total pseudo-first-order rate constant (per hr) for hydrolytic transformations of the toxicant in each compartment.	hr^{-1}
HYDRX	TOXIFORD	Intermediate calculation in obtaining temporally averaged concentration of hydroxide ions. HYDRX = 10**(-POHG)	unitless
I1, I2	TOXISEDW	Local variables representing segments involved in exchange. (See "IR(I), JR(I)" card group B).	unitless
ICHK	TOXIWASPB	Integer flag denoting day on which last set of daily flows and nonpoint source loads were read from auxiliary file. Saved in COMMON as TIMCHK.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
ICOUNT	TOXIDUMP	Number of entries into auxiliary file for statistical analysis. Integer value of TCOUNT.	unitless
ILCOL	TOXINIT	Subscript indicating column in table of daily flows from auxiliary file (1-10)	unitless
IL(J)	MAIN	Characteristic length for dispersive exchange, input in WASP2.	ft
INDEXS	TOXIWASPB TOXIFORD	INDEXS is an internally calculated flag designating a benthic compartment. INDEXS is 1 for benthic compartments (TYPEE = 3 or 4), 0 for water compartments (TYPEE = 1 or 2).	unitless
INDEXW	TOXIWASPB TOXIFORD	INDEXW is an internally calculated flag designating a water column compartment. It takes a value of 1 for water compartments (TYPEE = 1 or 2) and a value of 0 for benthic compartments (TYPEE = 3 or 4).	unitless
IOPT	TOXIDUMP	Flag designating type of output desired in TOXIDU.	unitless
ITCHK	TOXIWASPB TOXINIT	Integer flag denoting whether a full day has plassed since the last set of flows and nonpoint source loads were read from auxiliary file.	unitless
ITIMEC	TOXIWASPB	Integer flag denoting the current simulation day. The integer value of TIME	unitless
ITYPE	TOXINIT TOXISETL	Flag designating segment type. The integer value of TYPEE(J).	unitless
IZERO	TOXIPHOT	Light intensity at top of lower level water compartment, 0.0 to 1.0.	unitless
JROW	TOXINIT	Subscript indicating row in table of daily flows from auxiliary file.	unitless
JSTR	TOXIWASPB TOXINIT TOXIDUMP	Top bed segment below water segment FTR. Concentrations in JSTR are printed out during peak "events," and are saved every 3 hours on an auxiliary statistical file.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
JTR	TOXIWASPB TOXIDUMP	Segment used to trigger event printouts when total chemical concentration exceeds CTRIG. Saved in COMMON as XJTR. Concentrations in JTR are printed out during peak events, and are saved every 3 hours on an auxiliary statistical file.	
JL(J)	MAIN	Characteristic length for dispersive exchange input in WASP2.	ft
KAHG(I,1)	TOXIFORD	Second-order rate constants for specific-acid-catalyzed hydrolysis of toxicant. If the corresponding entry in the Arrhenius activation energy matrix (EAHG) for this reaction is zero, the value entered in KAHG is taken as the second-order rate constant. If the corresponding entry in the activation energy matrix (EAHG) is non-zero, the value entered in matrix KAHG is interpreted as the base-10 logarithm of the frequency factor in an Arrhenius function for the reaction, and local values (KAHL) of the second-order rate constant are computed as a function of temperature (TCELG) in each system compartment.	L/mole $[H^+]$-hr
KAHL	TOXIFORD	Local value of KAHG(I,1) corrected for temperature.	L/mole $[H^+]$-hr
KB	TOXIWASPB TOXIFORD TOXINIT	Effective biomass partition coefficient. Calculated internally by multiplying OCB and KOW.	L_w/kgb
KBACSG(I,1)	TOXIFORD	Second-order rate constants for benthic sediment bacterial biolysis of the organic toxicant. If the corresponding entry in the Q-10 matrix (QTBASG) for this process is zero, the number entered in matrix KBACSG is taken as the second-order rate constant. If the corresponding entry in the Q-10 matrix is non-zero, the value of the second-order rate constant at 20	ml/cell-hr

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
		degrees C., and local values (KGACSL) of the rate constant are computed as a function of temperature (BIOTMG) in each ecosystem compartment.	
KBACSL	TOXIWASPB TOXIFORD	Local value of KBACSG(I,1), corrected for temperature.	ml/cell-hr
KBACWG(I,1)	TOXIFORD	Second-order rate constants for water column bacterial biolysis of the toxicant. If the corresponding entry in the Q-10 matrix (QTBAWG) for this process is zero, the number entered in matrix KBACWG is taken as the second-order rate constant. If the corresponding entry in the Q-10 matrix is non-zero, the value entered in matrix KBACWG is interpreted as the numerical value KBACWL of the rate constant are computed as a function of temperature (BIOTMG) in each ecosystem compartment.	hr
KBACWL	TOXIWASPB	Local value of KBACWG(J), corrected for temperature.	mg/cell-hr
KBHG(I,1)	TOXIFORD	Second-order rate constants for specific-base-catalyzed hydrolysis of toxicant. If the corresponding entry in the Arrhenius activation energy matrix (EBHG) for this reaction is zero, the value entered in KBHG is taken as the second-order rate constant. If the corresponding entry in the activation energy matrix (EBHG) is non-zero, the value entered in matrix KBHG is interpreted as the base-10 logarithm of the frequency factor in an Arrhenius function for the reaction, and local values (KBHL) of the second-order rate constant are computed as a function of temperature (TCELG) in each system compartment.	L/mole [OH-]-hr
KBHL	TOXIWASPB TOXIFORD	Local value of KBHG(I,1), corrected for temperature.	L/mole [OH-]-hr

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
KDPG	TOXIFORD TOXIPHOT	A near-surface photolytic rate constant for the toxicant. The value of KDPG represents the outcome of an experiment conducted in natural sunlight. The constant is a temporally averaged (e.g., over whole days, seasons, etc.) first-order photolytic transformation rate constant pertaining to cloudless conditions at some reference latitude RFLATG.	hr^{-1}
KDPL	TOXIFORD TOXIPHOT	Locally adjusted value of KDPG returned from TOXIPHOT.	unitless
KNHG(I,1)	TOXIFORD	Rate constants for neutral hydrolysis of organic toxicant. If the corresponding entry in the Arrhenius activation energy matrix (ENHG) for this reaction is zero, the value entered in KNHG is taken as the rate constant. If the corresponding entry in the activation energy matrix (ENHG) is non-zero, the value entered in matrix KNHG is interpreted as the base-10 logarithm of the frequency factor in an Arrhenius function for the reaction, and local values (KNHL) of the rate constant are computed as a function of temperature (TCELG) in each system compartment.	hr^{-1}
KNHL	TOXIFORD	Local value of KNHG(I,1), corrected for temperature.	hr^{-1}
KO2G(J)	TOXIWASPB TOXINIT TOXIVOLT	Reaeration parameter at 20 degrees C in each ecosystem compartment. Calculated from segment depths and velocities, and time-varying wind.	cm/hr
KO2L	TOXIWASPB TOXIVOLT	Reaeration parameters in each compartment after temperature adjustment and units conversion.	m/hr
KOC	TOXIWASPB TOXINIT	Organic carbon partition coefficient. Value of KOC read in or if equal to zero, calculated from KOW. Multiplication of KOC by the fractional organic carbon content (OCS) of each	L_w/kg organic carbon

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
		system sediment yields the partition coefficient for sorption of unionized (SH2) compound to the sediment.	
KOW	TOXIWASPB TOXINIT	Octanol water partition coefficient. Value of KOW read in, or if equal to zero, calculated from KOC.	L_w/Loct
KOXG(I,1)	TOXIFORD	Second-order rate constants for oxidative transformation of toxicant. If the corresponding entry in the Arrhenius activation energy matrix (EOXG) for this reaction is zero, the value entered in KOXG is taken as the second-order rate constant. If the corresponding entry in the activation energy matrix (EOXG) is non-zero, the value entered in matrix KOXG is interpreted as the base-10 logarithm of the frequency factor in an Arrhenius function for the reaction, and local values (KOXL) of the second order constants are computed as function of temperature (TCELG) in each system compartment.	L/mole environmental oxidant/hr
KOXL	TOXIFORD	Local value of KOXG(I,1), corrected for temperature.	L/mole environmental oxidant/hr
KP(J)	TOXIWASPB TOXINIT TOXISETL	Effective sediment partition coefficient. Internally calculated as the product of KOC and OCS(J), and saved as Parameter 12.	L_w/kgs
KT	TOXINIT	Daily counter for reading nonpoint source loads from auxiliary tape and printing table (1-1000).	day
KVOG	TOXIVOLT	Measured experimental value for (volatilization) liquid-phase transport resistance, expressed as a ratio to the reaeration rate.	unitless
K20	TOXIFORD TOXIREOX	The computed reaeration rate at 20°C. Used to calculate the chemical volatilization rate.	day^{-1}

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
LATG	TOXIPHOT	Geographic latitude of ecosystem.	degrees
LIGHTL	TOXIPHOT	The average light intensity in the current compartment, as a fraction of the near-surface light intensity (taken as 1.0 or 100%).	unitless
LIGHTN	TOXIWASPB TOXIPHOT	Normalized light time function, transferred through COMMON as constant 78 to TOXIPHOT. There it adjusts the average photolysis rate for seasonal light variability.	unitless
LOPT	TOXIWASPB TOXINIT	Option to read in flows and/or nonpoint source loads on a daily basis: 0 = skip daily read option 1 = read sequential tape containing daily flows and/or loads	unitless
MOQ	TOXIWASPB TOXINIT	Number of flow pairs read from auxiliary file daily. MOQ is read from auxiliary file by TOXINIT and passed to TOXIWASPB through COMMON as the floating point variable MOQS.	unitless
MOQS	OXIWASPB TOXINIT	Number of flow pairs read from auxiliary file daily. MOQS is set equal to MOQ in TOXINIT and saved in COMMON as constant 83.	unitless
MQOPT	TOXINIT	Flow option read from auxiliary file. Not used.	unitless
MTYPE	TOXINIT	Flag designating type of segment immediately above current segment. Integer value of TYPEE(J-1).	unitless
MWTG	TOXIVOLT	The molecular weight of the toxicant.	g/mole
NCOL	TOXINIT	Variable indicating the number of column entries in the last row of daily flows from auxiliary file.	unitless
NOWKS	TOXIWASPB TOXINIT	Number of nonpoint source loads read from auxiliary file daily. NOWKS is read from auxiliary file by TOXINIT and passed to TOXIWASPB through COMMON as constant 84.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
NPSWK(I,J)	TOXIWASPB TOXINIT	Nonpoint source load J for constituent I (chemical or sediment), read from auxiliary file daily. The segment into which load J discharges is defined in Card Group F: Forcing Functions.	lb/day
NWKS	TOXIWASPB TOXINIT	Number of nonpoint source loads read from auxiliary file daily. NWKS is the integer value of NOWKS.	unitless
OCB	TOXINIT	Organic carbon content of the compartment biomass as a fraction of dry weight. Coupled to KOW to generate biomass partition coefficient.	unitless
OCS(J)	TOXINASPB TOXINIT	Organic carbon content of sediments as fraction of dry weight. Parameter is coupled to KOC to generate the sediment partition coefficient as a function of a property of the sediment.	unitless
OXIDKL	TOXIFORD TOXIDUMP	Pseudo-first-order rate constants for oxidative transformation of toxicant.	hr^{-1}
OXRADG(J)	TOXIFORD	Molar concentration of environmental oxidants (e.g., peroxy radicals) in each ecosystem compartment.	moles/L
PCTWA(J)	TOXIWASPB	Percent water in bottom sediments of benthic compartments. PCTWA(J) should be expressed as the conventional soil-science variable (fresh/dry weight); all values must be greater than or equal to 1.	unitless
PERC	TOXISETL	Pore water percolation, calculated from the spatially-variable parameter WS(J) for type 4 (subsurface benthic) segments.	million ft^3/day
PERCMS	TOXISETL	Mass transport rate of dissolved chemical in pore water.	MCF/day .mgc/L_w)
PH	TOXIWASPB TOXIFORD	Hydrogen ion activity of segment being considered. Local value of PHG(J).	pH

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
PHG(J)	TOXIWASPB	Hydrogen ion activity. The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydronium ions [H3O+] in gram-molecules per liter.	pH
PHOTKL	TOXIFORD TOXIDUMP	Pseudo-first-order rate constant for photolytic transformation of the toxicant.	hr^{-1}
PHN	TOXIWASPB	Normalized time function for PH. Adjusts PHG(J) for seasonal variability.	unitless
POHN	TOXIWASPB	Normalized time function for POH. Adjusts POHG(J) for seasonal variability.	unitless
PNEXT	TOXIWASPB TOXIDUMP	Triggers event printout every 3 hours during peak event period. Local value of POHG(J).	unitless
POH	TOXIWASPB TOXIFORD	Hydroxide ion activity of segment being considered. Local value of POHG(J).	POH
POHG(J)	TOXIWASPB	Hydroxide ion activity. The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydroxide [OH-] ions in gram-molecules per liter.	pOH
POROS	TOXISEDW	Porosity of top bed segment, used in computing dispersive exchange between bed and water column. For computing dispersive exchange between two bed segments, POROS is the mean porosity.	L_W/L_T
PTIME	TOXIDUMP	Rounded-off value of TIME for output.	day
QT(I)	TOXINIT	Variable for temporary storage of daily flows from auxiliary file.	unitless
QTBASG(I,1)	TOXIFORD	Q-10 values for bacterial transformation (c.f. KBACSG) of organic toxicant in benthic sediments. The Q-10 is the increase in the second-order rate constant resulting from a 10 degree C temperature increase.	unitless

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
QTBAWG(I,1)	TOXIFORD	Q-10 values for bacterial transformation (c.f. KBACWG) of chemical in the water column of the system. Q-10 is the increase in the second-order rate constant resulting from a 10 degree C temperature increase.	unitless
QUANTG(I,1)	TOXIFORD	Reaction quantum yield in photolytic transformation of chemical. The quantum yield is the fraction of total quanta absorbed by the toxicant resulting in transformations. Separate values are provided for each molecular configuration of the toxicant in order to make assumptions concerning their relative reactivities readily available to the user.	unitless
RATEK	TOXIVOLT TOXIPHOT	Internally calculated rate returned from TOXIVOLT or TOXIPHOT to TOXIFORD for use as VOLKL or KDPL.	unitless
RESGAS	TOXIVOLT	Gas film resistance to volatilization.	hr/m
RESLIQ	TOXIVOLT	Liquid film resistance to volatilization.	hr/m
RFLATG	TOXIWASPB	Reference latitude for corresponding direct photolysis rate constant (c.f. KDPG).	40.72
RVOL(J)	TOXINIT TOXISETL	Reference volume at which the sediment compaction cycle is initiated for surface bed segment "J". RVOL(J) is computed in TOXINIT for each surface bed segment and is stored in location RVOL(J-1) [equivalenced to VVOL(J-1)]. RVOL(J) is the surface bed volume that will hold the mass of sediment contained in the upper two bed segments at time 0. RVOL(J) will be greater than the combined volume of the upper two bed segments at time 0 if the density of the second bed segment is greater than the top bed segment.	million ft^3

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
SCALQ	TOXINIT	Scale factor to convert daily flows from auxiliary file to cubic.	ft/sec
SED	TOXIWASPB TOXIDUMP TOXISETL TOXISEDW	Sediment concentration of segment being considered.	mgs/L_T
SEDCOL	TOXISEDW	Sediment concentration after conversion to internal units (kg/liter of water) in sediment compartment.	kg/L_W
SEDFAC	TOXIWASPB	Intermediate variable for determining fraction of chemical sorbed onto sediment phase of a segment.	unitless
SEDFL	TOXISEDW	Rate of sediment mixture to the surface of the bed, allowing sorption or desorption with the overlying water. Related to the dispersive exchange of water by the spatially-varying parameter DSPSED(J).	MCF_W/day $.mgs/L_W$
SETINS, SETOUS	TOXISETL	Sediment settling into or out of compartment. These variables are transferred to TOXIWASPD to hold the values until the next call to TOXISETL.	mgs/L_T-day
SETINC, SETOUC	TOXISETL	Chemical settling into or out of a compartment. Chemical can only settle when adsorbed to sediment. These variables are transferred to TOXIWASPD to hold the values until the next call to TOXISETL.	mgc/L_T-day
SEDW	TOXISEDW	Sediment concentration in water compartment above bed.	kg/L_T
SMASS	TOXISETL	Mass of dissolved chemical in the pore water squeezed from the surface bed segment to the water column during the compaction cycle.	MCF. mgc/L_W

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
SOLG	TOXIVOLT	Aqueous solubility of toxicant chemical species. If the corresponding value in ESOLG (c.f.) is zero, SOLG is interpreted as an aqueous solubility in mg/liter. If ESOLG is non-zero, SOLG is used in an equation describing the molar solubility of the toxicant species as a function of environmental temperature (TCELG), i.e., SOLL(mg/l) = 1000.*MWTG*10.**J(SOLG-(1000.*ESOLG/(2.303*R*(TCELG+273.15)))). Solubilities are used (inter alia) to limit the permissible external loadings of the toxicant on the system to values that generate final residual concentrations .LE. 50% of aqueous solubility (or 1.E-5M). This constraint is imposed in order to help ensure that the assumption of linear sorption isotherms is not seriously violated.	mg/L_T
SOLL	TOXIVOLT	Temperature-corrected aqueous solubility of chemical.	unitless
SVOL	TOXISETL	Volume of pore water squeezed from the surface bed segment to the water column during the compaction cycle. SVOL is the difference in volume between the surface bed segment before compaction and the top two bed segments after compaction.	million ft^3
TCELG,TKEL	TOXIWASPB TOXIFORD TOXIVOLT	Product of segment temperature TEMPM(J) and temperature function TEMPN. Immediately converted to Kelvin temperature (TKEL) from Celsius.	°C
TCOUNT	TOXINIT TOXIDUMP	Number of entries into auxiliary file for statistical analysis. Stored in COMMON as constant 73.	unitless
TDINT	TOXIWASPB TOXIDUMP	Time interval between recalculation of decay rates.	day
TEMPM(J)	TOXIWASPB	Average temperature for compartment.	°C

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
TEMPN	TOXIWASPB	Value of normalized time function describing temperature. Multiples TEMPM to give TCELG.	unitless
TIMCHK	TOXIWASPB TOXINIT	Day on which last set of daily flows and nonpoint source loads were read from auxiliary file. Saved in COMMON as constant 82.	day
TMARK	TOXIWASPB TOXINIT	Day on which rate constants will be recalculated. Incremented throughout simulation by TDINT.	day
TMASS	TOXISETL	Mass of chemical transferred to the next lower bed segment during the compaction cycle. TMASS is first set to the mass of chemical in the top bed layer that is compacted into the new second bed layer (FVOL*CHEM). Once the new concentration of the second bed layer is determined, TMASS is set to the mass of chemical in the second bed layer that is buried into the new third bed layer. This is continued to the bottom bed segment, where TMASS is added to BMASS(J), the amount of chemical mass lost from the network by burial below segment J.	MCF. mgc/L_T
TMPM	TOXIWASPB TOXINIT	Temporarily held value of TMASS, the amount of chemical transferred to the next lower bed segment during the compaction cycle.	MCF. mgc/L_T
TOTKG(J)	TOXIWASPB TOXINIT	Total first order decay rates calculated externally. If equal to zero, the program evaluates all separate processes and calculates a combined total first order decay rate, TOTKL.	day^{-1}
TOTKL	TOXIWASPB TOXIFORD TOXIDUMP	Value of total first-order decay rate for compartment, derived from TOTKG (J).	day^{-1}
TQ	TOXIWASPB	Temporary value for flow or exchange between two segments, used for maximizing time step to minimize numerical dispersion and simulation cost.	ft^3/day

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
TRT	TOXIWASP	Test value of time step that would eliminate numerical dispersion in a segment.	days
TYPEE(J)	TOXIWASPB TOXINIT TOXIFORD TOXIPHOT TOXISETL TOXISEDW	Numerical code designating segment types used to define ecosystem. Available types: 1 = Epilimnion, 2 = Hypolimnion, 3 = Benthic (active), and 4 = Benthic (buried).	unitless
TYP1,TYP2	TOXISEDW	Internal variables describing type (e.g., TYP1 - TYPEE(I1)) of interchanging compartments.	unitless
V1,V2,...,V8	TOXIWASPB TOXIDUMP	Dummy variables used in argument of calls to TOXIDU.	unitless
VAPRG	TOXIVOLT	Vapor pressure of compound. Used to compute Henry's Law constant if the latter input datum (HENRYG) is zero, but VAPRG is non-zero.	torr, or mm Hg
VAPRL	TOXIVOLT	VAPRL is the converted value to atmospheres.	
VELOC(J)	TOXIWASPB TOXINIT	Average velocity of water in the compartment.	ft/sec
VOL	TOXIWASPB	Equal to BVOL(J), the volume of the compartment.	million ft^3
VOLKL	TOXIDUMP TOXIFORD	Pseudo-first-order rate constants for volatilization losses from surface water compartments.	hr^{-1}
VVOL(J)	TOXIWASPB TOXIFORD TOXISETL	A dummy array to hold parameters describing the varying surface bed segment volume.	unitless
WAT	TOXIVOLT	Piston velocity term for water vapor.	unitless
WATFL	TOXISEDW	Dispersive exchange of water between top bed segment and water column, or between two vertically adjacent bed segments.	ft^3/day

VARIABLE	FOUND IN SUBROUTINE	DEFINITION	UNITS
WIND	TOXIWASPB TOXIVOLT	Local, time-varying wind speed. Equal to the average wind velocity over a segment WINDG(J) times the time function WINDN.	m/sec
WINDG(J)	TOXIWASPB	Average wind velocity at a reference height of 10 cm above the water surface. Parameter is used to compute a piston velocity for water vapor (Liss 1973, Deep-Sea Research 20:221) in subroutine VOLAT.	m/sec
WINDN	TOXIWASPB	Normalized wind speed as function of time.	unitless
WS(J)	TOXISETL	Spatially variable parameter denoting settling rate of suspended sediment in water column segments (types 1 and 2), erosion rate of surface bed sediment in surface bed segment (type 3), or percolation of pore water through subsurface bed segments (type 4). Segment types 1,2: meters per day Segment type 3: cm per year Segment type 4: cubic feet/sec	
XJSTR	TOXIWASPB TOXINIT TOXIDUMP	Reference segment for triggering event and frequency output. A value of zero will disable it. A non-zero value will cause printout of all segment concentrations when the concentration at XJTR is greater than CTRIG. Also, a time history of concentrations (every 3 hours) at XJTR and its associated benthic segment will be stored for later frequency analysis.	unitless
XMASS	TOXIDUMP	Mass of chemical in segment.	kg
XXX	TOXIPHOT	Exponential light disappearance term.	unitless
XTES	TOXIPHOT	Maximum light disappearance term. After this value (87.4) no light is present.	unitless
XTST	TOXINIT TOXIDUMP	Test variable to determine whether to set up event-triggered printout. If either CTRIG or JTR is zero, then event-triggered printout is disabled.	unitless

SECTION 3

WASP3 PROGRAMMER'S MANUAL

3.1 OVERVIEW

This section is designed to supply information to familiarize the user with the programming aspects of the models. This section should facilitate making any desired modifications to the model and linking user defined kinetic subroutines.

3.2 THE HYDRODYNAMIC MODEL

3.2.1 Hardware and Software Requirements

3.2.1.1 Minimum Operational System--

PC Requirements--The execution of DYNHYD3 on a personal computer requires the following environment:

Storage Requirements:

Random Access Memory - 256K bytes

Diskette Drive - Required for installation only

Hard Disk Drive - 5 megabyte or larger

Installation Size - Approximately 440K bytes

DOS Version - 2.12 or higher

Numerical Coprocessor - 8087 or 80287 required

Dot Matrix Printer - 132 column capability.

Although the program is small enough to run on a single floppy drive, DYNHYD3 uses a scratch file that requires more space than afforded by a floppy disk.

VAX requirements--Since the development and improvement of DYNHYD3 have been processed on a Digital Computer, the program requirements will be discussed for a VAX 11/785 only. In addition, DYNHYD3 requires the use of approximately 10,000 blocks of hard storage, which increases proportionally with the length of simulation and number of time steps. This large disk usage can be attributed to a scratch file containing preliminary and final calculations of the simulation.

3.2.1.2 Development System--

The DYNHYD3 program was ported to the personal computer environment using the following software development tools.

Language: FORTRAN 77

Operating System: PC DOS 3.1

Compiler: IBM Professional FORTRAN (PROFORT) V1.0

Linkage Editor: IBM Professional FORTRAN (LINK) V2.3

The selection of IBM's Professional FORTRAN (PROFORT) was due to its close adherence to the ANSI FORTRAN Standards. These standards allow for a pure transportable code for other machines and compilers.

3.2.2 Installation and Implementation

3.2.2.1 Personal Computer--

Installation of DYNHYD3 onto a personal computer requires the following steps:

Description	Command
1. Set the default drive to the hard disk (e.g., hard disk "n"):	`n:`
2. Create a DYNHYD3 sub-directory:	`MKDIR DYNHYD3`
3. Change default directory:	`CD/DYNHYD3`
4. Transfer files from diskette (e.g., drive "m") to the hard disk with verification of copy.	`COPY m:*.* n:*.* /V`
5. Verify copy by listing directory contents:	`DIR`

The following is a brief description of all files contained on the distribution diskettes.

README.1ST - Document containing the following list.

DYNHYD3.FOR - The FORTRAN source code file for the DYNHYD3 program.

DHYD.COM - The COMMON block source code included in the main source code by the FORTRAN INCLUDE statement.

DYNHYD3.EXE - The executable task image.

COMPLINK.BAT - A batch command file that compiles and link edits the DYNHYD3 program.

DYNHYD.BAT - A batch command file that executes DYNHYD3. To execute, type: DYNHYD3 "file name" where "file name" is the name of the input data set (ex. DYNHYD3 COEF2.INP).

COEF2.INP - A data set that may be used as input for the DYNHYD3 model for testing the installation of the DYNHYD3 system. COEF2.INP is a simple hydrodynamic estuary for a 13 segment network.

COEF2.OUT - A sample output file created by running the input data set, COEF2.INP. Comparison of the created DYNHYD3.OUT to COEF2.OUT will demonstrate the model's working order.

CANAL.INP
CANAL.OUT - An input and output data set that provides an linkage example of DYNHYD3 to WASP3V2.

CANAL.INP - An input data set for EUTRWASP. This data set requires the hydrodynamic input of SUMRY2.OUT which is created by DYNHYD3 and COEF2.INP.

Note

Linkage requires the following switches:

-COEF2.INP must have a "2" in column five of the SUMMARY CONTROL DATA card group. (This modification has been included.)

-CANAL.INP must have a "5" in line one, column five of card group D. This indicates to WASP3V2 to read volumes and flows from a previously created file (by DYNHYD3) called SUMRY2.OUT.

The executable task image DYNHYD3.EXE for the IBM PC and compatible systems has been included on distribution diskettes. The IBM Professional FORTRAN compiler and linkage editor (PROFORT and LINK) are not required to run the DYNHYD3 program. If any modification of the FORTRAN source code is desired, however, then both of these software development tools will be required.

3.2.2.2 VAX--

See Section 3.3.2 (WASP installation procedures).

3.2.3 Description of VAX Command Files

Description:

DYNCOMP.COM - This command file compiles , links and executes the DYNHYD3 program. The command procedure selects the appropriate source code and common blocks needed to build the DYNHYD3 task image. To run this program on the VAX, type:

```
@DYNCOMP INPUTFILE.NAME
```

where "INPUTFILE.NAME" is the input data file.

Listing:

```
$!*********************************************************************
$!*        THIS COMMAND FILE WILL WORK ON A VAX SYSTEM UNDER VMS      *
$!*                                                                   *
$!*         Command file to compile, link and execute DYNHYD3         *
$!*      To use this command file type:                               *
$!*                                                                   *
$!*                    @DYNCOMPILE INPUTFILE.NAME                     *
$!*                                                                   *
$!*      Where INPUTFILE.NAME is the file in which you would like     *
$!*      to have executed by DYNHYD3.  This follows the standard      *
$!*      parameter statement described by the VMS manual.  To submit  *
$!*      a batch job type:                                            *
$!*                                                                   *
$!*            SUB/PARA=(INPUTFILE.NAME) DYNCOMP                      *
$!*                                                                   *
$!*********************************************************************
$!
$!                                  ***********************************
$ SET DEF [EXAMPLE.WASP]! <---------* Change default to appropriate   *
$!                                  * directory                       *
$!                                  ***********************************
$!
$ DEFINE/USER_MODE  INFILE 'P1'
$!
$ COPY INFILE DYNHYD3.INP!  INFILE IS EQUAL TO THE INPUT FILE
$!                          DEFINED TO RUN TEST CASE
$ FO DYNHYD3
$!
```

```
$!
$ LINK DYNHYD3
$!
$ DEL DYNHYD3.OBJ;*
$!
$!
$ RUN DYNHYD3
$!
$ PRINT DYNHYD3.OUT
$!
$ PURGE RESTART.OUT
$ PURGE DYNHYD3.OUT
$ PURGE SUMRY2.OUT*
$ PURGE *.LIS
$ DEL DYNHYD3.INP;*
$ DEL SCRATCH.TMP;*
```

Description:

DYNRUN.COM - This command file executes the DYNHYD3 task image with any user supplied input data stream. To use DYNRUN.COM type:

```
@DYNRUN INPUTFILE.NAME
```

Listing:

```
$!*********************************************************************
$!*        THIS COMMAND FILE WILL WORK ON A VAX SYSTEM UNDER VMS      *
$!*                                                                   *
$!*                 Command file to execute DYNHYD3                   *
$!*                To use this command file type:                     *
$!*                                                                   *
$!*                   @DYNRUN INPUTFILE.NAME                          *
$!*                                                                   *
$!*      Where INPUTFILE.NAME is the file to be executed by           *
$!*      DYNHYD3.  This follows the standard parameter statement      *
$!*      described by the VMS manual.  To submit a batch job to       *
$!*      do the same thing type:                                      *
$!*                                                                   *
$!*           SUB/PARA=(INPUTFILE.NAME) DYNRUN                        *
$!*                                                                   *
$!*********************************************************************
$!
$!                                  ***********************************
$ SET DEF [EXAMPLE.WASP]! <---------* Change default to appropriate   *
$!                                  * directory                       *
$!                                  ***********************************
$ DEFINE/USER_MODE  INFILE 'P1'
$ COPY INFILE DYNHYD3.INP!
$!
$ RUN DYNHYD3
```

```
$!
$ PRINT DYNHYD3.OUT
$!
$ PURGE RESTART.OUT
$ PURGE DYNHYD3.OUT
$ DEL DYNHYD3.INP;*
$ DEL SCRATCH.TMP;*
```

3.2.4 Description of Computer Program

3.2.4.1 Overview of Systems--

Figure 52 is a flow chart of DYNHYD3 illustrating the functional relationships among the subroutines. The main program opens files, calls DYNHYD, closes files, and calls the post-processor subroutines that create the saved output files. Subroutine DYNHYD accomplishes the data input simulation, and printed output, with assistance from SEAWRD, REGAN, WIND, and RUNKUT.

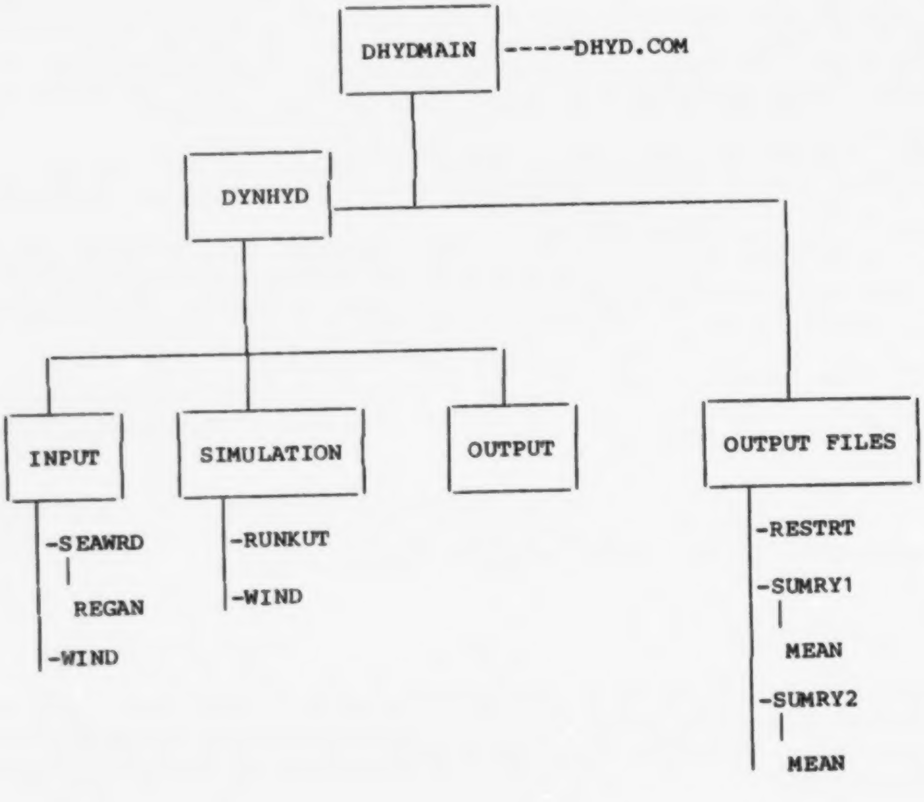

DHYDMAIN
-----DHYD.COM
DYNHYD
INPUT
-SEAWRD
REGAN
-WIND
SIMULATION
-RUNKUT
-WIND
OUTPUT
OUTPUT FILES
-RESTRT
-SUMRY1
MEAN
-SUMRY2
MEAN

Figure 52. DYNHYD3 flow chart.

DYNHYD3 INPUT/OUTPUT UNITS

All the input/output units used in DYNHYD3 are controlled by definable variables. These variables are in the global common block DHYD.COM and can easily be reassigned. The individual units are listed below with their default integer values. A brief description is provided to illustrate how the units are used within the program.

ICRD: User must specify 5 or 8. File 5 refers to the input data set DYNHYD3.INP. An 8 denotes the input data stream is in File 8. File 8 is created from File 9 and contains a snapshot of the final conditions from the previous run (created by the subroutine RSTRT). Files 5 and 8 are formatted sequential files. Example: READ(ICRD).

IN: Default value is 5. The value 5 denotes the input data stream is in DYNHYD3.INP. The input data stream is a formatted sequential file. Example: READ(IN).

MESS: Default value is 6. Mess has been implemented mainly for the personal computer but may be of some benefit for the main frame user as well. MESS allows runtime status messages to be displayed on the screen, and allows the user to track where in the simulation program execution is occurring. Please note that MESS must always be assigned unit 6 or it will not default the messages to the screen but to a FOR000.DAT file. File 6 is a formatted sequential file. Example: WRITE(MESS).

OUT: The default value is 1. File 1 is the output file called DYNHYD3.OUT. File 1 is a formatted sequential file. Example: WRITE(OUT).

RSTR: The default value is 9. File 9 contains a snapshot (flows and volumes) of the final conditions of a run. File 9 will be converted to File 8, an input stream for the next run. File 9 is a formatted sequential file. Example: WRITE(RSTR).

SCR: The default value is 2. File 2 is the scratch file processed by the subroutine SUMRY1 (or 2). File 2 is an unformatted sequential file. Example: READ and WRITE(SCR).

SUMY: The default value is 4. File 4 is the SUMRY file containing flows and volumes used by the water quality model. File 4 is a formatted or unformatted sequential file. Example: WRITE(SUMY).

3.2.4.2 Common Block--

DYNHYD3 has a common block transferred between subroutines. This common block consists of nine sections that are grouped according to subject matter. The following is a listing of the common block, plus the variables associated with each section:

```
 COMMON /CHAN/ AK(CH), AREA(CH), AREAT(CH), B(CH), CLEN(CH),
*              CN(CH), NJUNC(CH,2), Q(CH), R(CH), V(CH),
*              VT(CH),CDIR(CH)
 COMMON /JUNC/ JPRT(JU), NCHAN(JU,5), SURF(JU), VOL(JU),
*              Y(JU), YT(JU), QIN(JU),BELEV(JU)
 COMMON /VFLO/JRVF(VF), NINCR(MQ), NQ(MQ), NVFLOW, QCYC(VF,MQ),
               VFLOW(VF,MQ), VQIN(JU), VQ(VF,JU)
 COMMON /CFLO/ CQIN(JU), NCFLOW, JRCF(CF), CFLOW(CF)
 COMMON /SEA/  A1(SB,7), PERIOD(SB), NS, NK, NSEA, NINL, RANGE(SB),
*              BTIME(SB,TC2), BHEAD(SB,TC2), NTV(SB), NHCYC(SB),
*              DTIME(SB),TREP(SB),TSTART(SB)
 COMMON /TIME/ DELT, DT, DT2, T, T2, TEND, TZERO, TTIME(SB)
 COMMON /MISC/ ALPHA(80), G, ICYC, NJ, NC, NCYC, W(SB), MOM(CH),
*              FRIC(CH), GRAV(CH), WIN(CH)
 COMMON /FILE/ SUMRY,ITAPE,LTAPE,ICRD,NODYN
 COMMON /WIND/ WINDS(MQ), WDIR(MQ), NOBSW, IW, WTIM(MQ), FW(CH),
*              IREADW, WSLOPS, WSLOPA, TREPW, DTIMW
```

The COMMON "CHAN" refers to all variables associated with channels. The "COMMON "JUNC" refers to all variables associated with junctions. The COMMON "VFLO" refers to all variables associated with variable inflows. The COMMON "CFLO" refers to all variables associated with constant inflows. The COMMON "SEA" refers to all variables associated with seaward boundaries. The COMMON "TIME" refers to all variables associated with the time step. The COMMON "MISC" is a collection of miscellaneous variables. The COMMON "FILE" refers to input/output fields. The COMMON "WIND" refers to all variables associated with the wind.

In each common, the dimensions of a variable are defined by parameters. The value of these parameters are also defined in a common block called "DHYD.COM." The separation of these parameters allows easy alterations. The following is a list of parameter definitions.

JU = number of junctions

CH = number of channels

VF = number of variable inflows

CF = number of constant inflows

ND = number of time steps per quality time steps

MQ = maximum number of flow or wind values in time function

NR = ND + 1

SB = number of seaward boundaries

TC = maximum number of tidal cycles.

3.2.4.3 Subroutine Descriptions--

The following is a brief explanation of each subroutine function contained in DYNHYD3:

DHYDMAIN

The DHYDMAIN subroutine is the control module. It assigns input and output unit numbers, and operates the calling sequence for the input, simulation, and output subroutines.

DYNHYD

DYNHYD reads the majority of the input data: program description cards (Data Group A), program control data (A), output control data (B), hydraulic summary data (C), junction data (D), channel data (E), and inflow data (F). Subroutines WIND and SEAWRD are called to read the observed wind conditions, and seaward boundary data, respectively. DYNHYD calls the simulation (processing) subroutines: WIND and RUNKUT for each time step. Information is printed and the following values are initialized: constants, junction volumes, the scratch file, counters, and variables.

SEAWRD

SEAWRD has three options for reading the observed seaward boundary data. The first option reads the regression coefficients directly for the average tide. The second option calls REGAN to compute the average tide regression coefficients from average observed tidal heights versus time. The third option reads variable (highs and lows) observed tidal heights versus time and fits a repetitive one-half sine wave to the data points.

WIND

WIND has two sections. The first section, entered only once at the beginning of the simulation, reads in wind speed and direction versus time and sets up two piecewise linear functions of time. The second section updates the wind speed and direction by linear interpolation and calculates the wind accelerational force.

REGAN

REGAN, called by SEAWRD, performs a least squares fit to the observed seaward boundary data to describe an equation of the form:

$$Y(T) = A1 + A2\ \sin(\omega t) + A3\ \sin(2\omega t) + A4\ \sin(3\omega t) +$$

$$A5\ \cos(\omega t) + A6\ \cos(2\omega t) + A7\ \cos(3\omega t)$$

by solving normal equations.

RUNKUT

RUNKUT solves the equations of continuity and momentum using a modified Runge-Kutta technique. Channel velocity, channel flow, junction heads, junction volumes, and channel cross-section are computed for every half time step and every full time step. RUNKUT also checks stability of the system and exits program if the channel velocity exceeds 20 ft/sec.

RESTRT

As a start-up for the next run, RESTRT produces a snapshot of the current run's final conditions. At the end of the simulation, the title, variable trstrt, variable nrstrt, junction information (number, head, surface area, flow, and connecting channels), and channel information (number, length, width, surface area, Manning roughness coefficient, velocity, and hydraulic radius) are written to file RSTR.

SUMRY1 and SUMRY2

SUMRY1 and SUMRY2 summarize and save a record of the hydraulic conditions. Hydraulic parameters are saved with a frequency dependent on the lengths of the hydraulic time step and the time step used in the water quality model accessing the stored hydraulic data. The parameters stored for use by the quality model (see Figure 53) are junction volumes and inflows, channel flows, velocities, and depths. SUMRY1 creates an unformatted file and SUMRY2 creates a formatted file. For averaging flows, velocities and depths SUMRY calls MEAN.

MEAN

MEAN computes the average junction volumes and inflows, channel flows, velocities, and depths over a time step (DELTQ) equal to the hydraulic time step (DELT) times the water quality time step (NODYN) divided by 3600 seconds: DELTQ = DELT * NODYN/3600. MEAN is capable of three averaging options: Simpson's transformation, trapezoidal transformation, and straight transformations. At the present, MEAN is hardwired to use the trapezoidal transformation.

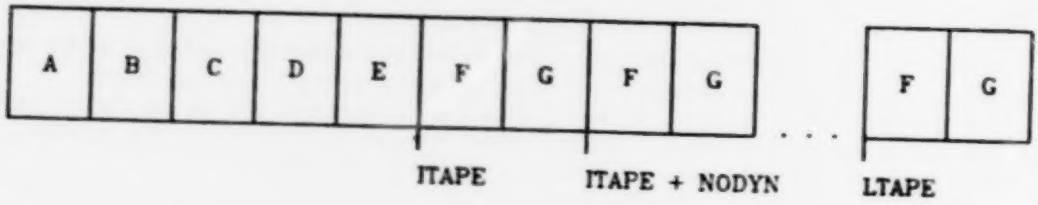
3.3 THE BASIC WATER QUALITY MODEL

3.2.1 Hardware and Software Requirements

3.3.1.1 Minimum Operational System--

Personal Computer Requirements

The size and structure of the WASP program require the following personal computer environment:



A) ALPHA(1-40), NJ, NC, DELT, ITAPE, LTAPE, SUMRY, NODYN (CLEN(N), B(N), CN(N)(NJUNC(N,I) I=1,2) N=1,NC)
Title, Network Size, Time Interval, Beginning Cycle, End Cycle, Tape Format, Number Hydraulic Time Steps per Qualtiy Time Step, Length of Channel, Width of Channel, Lower or Higher Junction Designator

B) ((SURF(J), NCHAN(J,K) K=1,5) J=1,NJ)
Surface Area of Junction, Channel Number Entering Junction

C) NCFLOW (JRCF(I), CFLOW(I) I=1,NCFLOW)
Number of Constant Flow Inputs, Junction Receiving Constant Flow, Constant Inflow + or −

D) NVFLOW (JRVF(I), NINCR(I) I=1,NVFLOW)
Number of Variable Flows, Number of Increments in Variable Flow

E) (QCYC(I,K) (VFLOW(I,K) K=1,NI) I=1,NVFLOW)
Hydrodynamic Cycle (Time Step), Flow value for Variable Flow

F) CYCLE, (VOL(J), QINSAV(J) J=1,NJ)
Hydrodynamic Cycle, Volume of Junction, Inflow into Junction

G) (QSAVE(N), VSAVE(N), RSAVE(N) N=1,NC)
Average Flow, Average Velocity, Average Hydraulic Radius

Figure 53. Summary tape description.

- 640 kilobyte Random Access Memory (RAM)
- 360 kilobyte diskette drive
- 5/10/20 megabyte hard disk drive
- 8087 math coprocessor
- DOS version 2.12 or higher
- dot matrix printer with 132 column capability

These requirements refer to the distribution versions. Depending upon the user's specific simulation, the variables may need redimensioning, thus increasing the Random Access Memory (RAM) requirements.

VAX 11/785 Requirements

The VAX requires a minimum of 4000 blocks of disk space to build and execute the program.

3.3.1.2 Development System for the Personal Computer--

The WASP system of programs were ported to the personal computer environment using the following software development tools:

Language:	FORTRAN 77
Operating System:	PC DOS 3.1
Compiler:	IBM Professional FORTRAN (PROFORT) v1.0
Linkage Editor:	Phoenix Software Associates, LTD (PLINK86) v1.47

The selection of IBM's Professional FORTRAN (PROFORT) was due to its adherence to the ANSI Fortran Standards. The source code for the VAX 11/785 is exactly the same as the personal computer code.

Phoenix Software's PLINK86 was chosen because of its ability to overlay both code and data.

3.3.2 Installation and Implementation

Personal Computers:

Installation of the WASP system onto a personal computer requires the following steps:

Description	Command
Set the default drive to the hard disk (e.g., hard disk "n"):	`n:`
Create a WASP3P directory:	`MKDIR WASP3P`
Request verification of copy:	`VERIFY ON`
Change default directory:	`CD/WASP3P`
Transfer files from diskette (e.g., drive "m") to the hard disk:	`RESTORE m: n:`
Remove verification:	`VERIFY OFF`
Verify directory contents:	`DIR`

To test the execution of the program, test data sets have been supplied with corresponding outputs for comparisons.

The following is a brief description of all files contained on the distribution diskettes:

README.1ST - Document containing the following list.

COMPLINK.BAT - A batch command file to compile and link edit either the toxics or eutrophication WASP source code. See program for documentation.

TOXIWASP.BAT - A batch command file that executes TOXIWASP. To execute, type: TOXIWASP "file name" where "file name" is the name of an input data set (ex. TOXIWASP POND.INP).

EUTRWASP.BAT - A batch command file that executes EUTRWASP. To execute, type: EUTRWASP "file name" where "file name" is the name of an input data set (ex: EUTRWASP 2DLAKE.INP).

TOXIWSP3.LNK
EUTRWSP3.LNK - These are link edit command files used by the PLINK86 linkage editor in COMPLINK.BAT.

POND.OUT
2DLAKE.OUT - These are sample output files for TOXIWASP and EUTRWASP test runs using POND.INP and 2DLAKE.INP, respectively. Compare these to WASP.OUT after executing the appropriate version of the model.

POND.INP
2DLAKE.INP - Data sets that may be used as input for the TOXIWASP and EUTRWASP models to test the installation of the WASP system. POND.INP is a simple pond and sediment system in which toxic degradation and mobility are simulated. 2DLAKE.INP simulates eutrophication attributes in a stratified lake system.

WASP3V2.FOR - The FORTRAN source code for the WASP driver program. This program solves the mass balance equation and controls the time step function.

TOXIWASB.FOR - The kinetic subroutine linked with WASP3V2.FOR to simulate organic toxics.

EUO3WASP.FOR - The kinetic subroutine linked with WASP3V2.FOR to simulate eutrophication attributes.

TOXIWSP3.CMN
EUO3WSP3.CMN - See note below.

NOTE: If the user selects to compile and link edit WASP3V2 without using the batch command file COMPLINK.BAT as described above, then he will be required to either:

- Copy TOXIWSP3.CMN to WSPCMN.F4P before compiling WASP for organic toxics, or
- Copy EUO3WSP3.CMN to WSPCMN.F4P before compiling WASP for eutrophication simulation.

This is required due to the different FORTRAN common blocks for EUTRWASP and TOXIWASP. This step is needed when compiling WASP without using the batch command file COMPLINK.BAT. Using the command file, editing is required to select the appropriate common block to be copied for each compile and link edit (see COMPLINK.BAT for further detail).

EUO3WSPB.CMN
TOXIWSPB.CMN - The common blocks that are required by the kinetic subroutines (EUO3WASP.FOR and TOXIWASB.FOR).

TOXIWSP3.EXE
EUTRWSP3.EXE - The executable task image codes.

VAX INSTALLATION:

Installation of the WASP model onto the VAX system requires the following steps:

Description	Command
Mount the tape	MOU/NOASSIST/OVERRIDE=OWNER MSA0:WASP32
Set default to desired directory	Set Def DBA0:[xxx.yyy]
Copy contents	Copy MSA0:*.*;* DBA0:[xxx.yyy]
Check to see if files were copies	DIR
Dismount the tape	Dismount MSA0:

TOXICOMP.COM - This command file compiles, links and executes the TOXIWASP program. This procedure will select the appropriate source code and common blocks needed to build the TOXICS task image. To run this program on the VAX type:

```
                        @TOXICOMP INPUTFILE.NAME

                   where INPUTFILE.NAME is the input data file.
```

```
$!**********************************************************************
$!*        THIS COMMAND FILE WILL WORK ON A VAX SYSTEM UNDER VMS       *
$!*                                                                    *
$!*        Command file to compile, link and execute TOXIWASP          *
$!*                To use this command file type:                      *
$!*                                                                    *
$!*                    @TCOMPILE INPUTFILE.NAME                        *
$!*                                                                    *
$!*      Where INPUTFILE.NAME is the file to be executed by DYNHYD3.   *
$!*      This follows the standard parameter statement described by    *
$!*      the VMS manual.  To submit a batch job type:                  *
$!*                                                                    *
$!*            SUB/PARA=(INPUTFILE.NAME) TOXICOMP                      *
$!*                                                                    *
$!**********************************************************************
$!
$!                                   ***********************************
$ SET DEF [EXAMPLE.WASP]! <---------* Change Default to Appropriate   *
$!                                   * Directory                       *
$!                                   ***********************************
$ DEL WSPCMN.F4P;*
$!
$ DEL TOXI.FOR;*
$ CREATE TOXI.FOR
$!
$ COPY TOXIWSP3.CMN WSPCMN.F4P
$!
$ DEFINE/USER_MODE  INFILE 'P1'
$!
$ COPY INFILE WASP.INP
$!
$ APPEND WASP3V2.FOR TOXI.FOR
$ APPEND TOXIWASB.FOR TOXI.FOR
$!
$ FO TOXI.FOR
$!
$ LINK TOXI
$!
$ DEL TOXI.OBJ;*
```

For file description see personal computer installation and implementation Section 3.2.2.

3.3.3 Description of VAX Command Files

The following is a description and listing of each command file that compiles and link edits on the VAX 11/785 under VMS.

TOXIRUN.COM - This command procedure will execute the TOXICS task image with a supplied input data stream. To use TOXIRUN.COM type:

```
@TOXIRUN INPUTFILE.NAME
```

```
$!*********************************************************************
$!*       THIS COMMAND FILE WILL WORK ON A VAX SYSTEM UNDER VMS       *
$!*                                                                   *
$!*                  Command file to execute TOXIWASP                 *
$!*                   To use this command file type:                  *
$!*                                                                   *
$!*                       @TRUN INPUTFILE.NAME                        *
$!*                                                                   *
$!*     Where INPUTFILE.NAME is the file to be executed by DYNHYD3.   *
$!*     This follows the standard parameter statement described by    *
$!*     the VMS manual.  To submit a batch job type:                  *
$!*                                                                   *
$!*           SUB/PARA=(INPUTFILE.NAME) TOXIRUN                       *
$!*                                                                   *
$!*********************************************************************
$!
$!                                 ***********************************
$ SET DEF [EXAMPLE.WASP]! <---------* Change Default to Appropriate   *
$!                                 * Directory                       *
$!                                 ***********************************
$ DEFINE/USER_MODE  INFILE 'P1'
$ COPY INFILE WASP.INP
$!
$ RUN TOXI
$!
$ PRINT WASP.OUT
$!
$ PURGE RESTART.OUT
$ PURGE WASP.OUT
$ DEL WASP.INP;*
$ DEL FREQ.TMP;*
$!
$ DEL TOXI.FOR;*
$!
$ RUN TOXI
$!
$!
$ PURGE RESTART.OUT
$ PURGE WASP.OUT
$ DEL WASP.INP;*
```

EUTRORUN.COM - This command procedure executes the EUTRO task image with any supplied input data stream. To use EUTRORUN.COM type:

@EUTRORUN INPUTFILE.NAME

```
$!*******************************************************************
$!*        THIS COMMAND FILE WILL WORK ON A VAX SYSTEM UNDER VMS    *
$!*                                                                 *
$!*                Command file to execute EUTRO.                   *
$!*                To use this command file type:                   *
$!*                                                                 *
$!*                    @ERUN INPUTFILE.NAME                         *
$!*                                                                 *
$!*      Where INPUTFILE.NAME is the file to be executed by EUTRO.EXE. *
$!*      This follows the standard parameter statement described by *
$!*      the VMS manual.  To submit a batch job type:               *
$!*                                                                 *
$!*            SUB/PARA=(INPUTFILE.NAME) EUTRORUN                   *
$!*                                                                 *
$!*******************************************************************
$!
$!                               **********************************
$ SET DEF [EXAMPLE.WASP]! <---------* Change Default to Appropriate  *
$!                               * Directory                      *
$!                               **********************************
$ DEFINE/USER_MODE   INFILE 'P'
$ COPY INFILE WASP.INP
$!
$ RUN EUTRO
$!
$ PRINT WASP.OUT
$ PURGE RESTART.OUT
$ PURGE WASP.OUT
$ DEL WASP.INP;*
$ DEL FREQ.TMP;*
```

EUTROCOMP.COM - This command file compiles, links and executes the EUTROWASP program. This procedure will select the appropriate source code and common blocks needed to build the EUTRO task image. To run this program on the VAX type:

@EUTROCOMP INPUTFILE.NAME

```
$!*********************************************************************
$!*        THIS COMMAND FILE WILL WORK ON A VAX SYSTEM UNDER VMS      *
$!*                                                                   *
$!*        Command file to compile, link and execute EUTRWASP         *
$!*                To use this command file type:                     *
$!*                                                                   *
$!*                    @ECOMPILE INPUTFILE.NAME                       *
$!*                                                                   *
$!*      Where INPUTFILE.NAME is the file to be executed by EUTRWASP. *
$!*      This follows the standard parameter statement described by   *
$!*      the VMS manual.  To submit a batch job type:                 *
$!*                                                                   *
$!*            SUB/PARA=(INPUTFILE.NAME) EUTROCOMP                    *
$!*                                                                   *
$!*********************************************************************
$!
$!                                  ***********************************
$ SET DEF [EXAMPLE.WASP]! <---------* Change Default to Appropriate   *
$!                                  * Directory                       *
$!                                  ***********************************
$ DEL WSPCMN.F4P;*
$!
$ DEL EUTRO.FOR;*
$ CREATE EUTRO.FOR
$!
$ COPY EUO3WSP3.CMN WSPCMN.F4P
$!
$ DEFINE/USER_MODE  INFILE 'P1'
$!
$ COPY INFILE WASP.INP
$!
$ APPEND WASP3V2.FOR EUTRO.FOR
$ APPEND EUO3WASP.FOR EUTRO.FOR
$!
$ FO EUTRO.FOR
$!
$ LINK EUTRO
$!
$ DEL EUTRO.OBJ;*
$!
$!
$ RUN EUTRO
$!
$!
$ DEL EUTRO.FOR;*
$!
$  PRINT WASP.OUT
$!
$ PURGE RESTART.OUT
$ PURGE WASP.OUT
$ DEL WASP.INP;*
$ DEL FREQ.TMP;*
```

*******************NOTE*****************

If it is desired to use the above command files in a batch mode simply type:

```
SUB/PARA=(INPUTFILE.NAME) COMMAND FILE NAME

EX:  SUB/PARA=(POND.INP) TOXIRUN OR TOXICOMP
```

3.3.4 Description of Computer Program

3.3.4.1 Overview of System--

Input/Output Files

All the input/output units can be reassigned an integer value in the WASP MAIN subroutine. It is suggested that the new user not change these units until he becomes more familiar with the structure and function of the program. The following is a brief description of each integer and their default integer values.

AUX: Default value is 4. AUX refers to the use of an auxiliary flow file. This file has been created outside the WASP programs and is used to input flows and volumes. Example: READ(AUX).

HYDRO: Default value is 7. HYDRO is the input data set created by DYNHYD3 (SUMRY1.OUT or SUMRY2.OUT). This file contains flows and volumes calculated by DYNHYD3. HYDRO is a sequential formatted (SUMRY1.OUT) or unformatted (SUMRY2.OUT) file. Example: READ(HYDRO).

IN: Default value is 2. The value 2 refers to the input data set. Input data set is a sequential formatted file. May also be used to represent the integer 2. Example: READ(IN).

OUT: Default value is 5. OUT refers to the output file "WASP.OUT." OUT may also represent the integer 5. WASP.OUT is a sequential formatted file. Example: WRITE(OUT).

RESRT: Default value is 9. RESTRT refers to the file containing a snapshot of final conditions. This file may then be used as initial conditions in the next run. RESTRT is a sequential formatted file. Example: WRITE(RESTRT).

SCRN: Default value is 6. Implemented for the benefit of the PC version, SCRN is designed to give screen messages to user indicating stage of simulation and execution. SCRN may be helpful to both the PC and mainframe user because it can act as a diagnostic file. SCRN can illustrate where program termination occurred. To examine SCRN type of list "SCREEN.OUT." "SCREEN.OUT is a sequential formatted file. Example: READ(SCRN).

Figure 54 is a flow chart of WASP3 illustrating the functional relationships among the subroutines. The main program opens files, calls the input, simulation, and output subroutines, and closes files. The input subroutines are called sequentially, as shown. Subroutine EULER controls the actual simulation, calling DERIV each time step to recalculate mass derivatives. The output subroutines are called sequentially as shown after the simulation is completed. The utility subroutines can be called by the other subroutines as needed.

3.3.4.2 Common block

****** WASP COMMON BLOCK ******

The WASP program requires two "include" common blocks that are brought into the program during compilation of the program. These common blocks are the WASP DRIVER common block (WSPCMN.F4P) and the KINETIC subroutine common block (TOXIWSPB.CMN or EUO3WSPB.CMN). The WASP DRIVER common block consists of five distinct groups: parameters, integers, real numbers, labelled files and intermediate files. The parameter statement found at the top of the WASP DRIVER common block dimensions arrays variables. The common block included into the WASP DRIVER program depends on the model: TOXIWASP or EUTRWASP. The batch command files that are supplied with the distribution tapes or diskettes will include the appropriate common block for TOXIWASP or EUTRWASP.

COMMON BLOCKS

TOXIWSP3.CMN

EUO3WSP3.CMN - See note below.

NOTE: If the user selects to compile and link edit WASP3V2 without using the batch command files EUTRO COMP.COM or TOXICOMP.COM, he must either:

- copy TOXIWSP3.CMN to WSPCMN.F4P when compiling WASP for organic toxics, or
- copy EUO3WSP3.CMN to WSPCMN.F4P when compiling WASP for eutrophication simulation.

EUO3WSPB.CMN - The common block used for the Eutrophication kinetic subroutine.

TOXCMN.F4P - The common block used for the Toxics kinetic subroutine.

The following is a listing of the three common blocks.

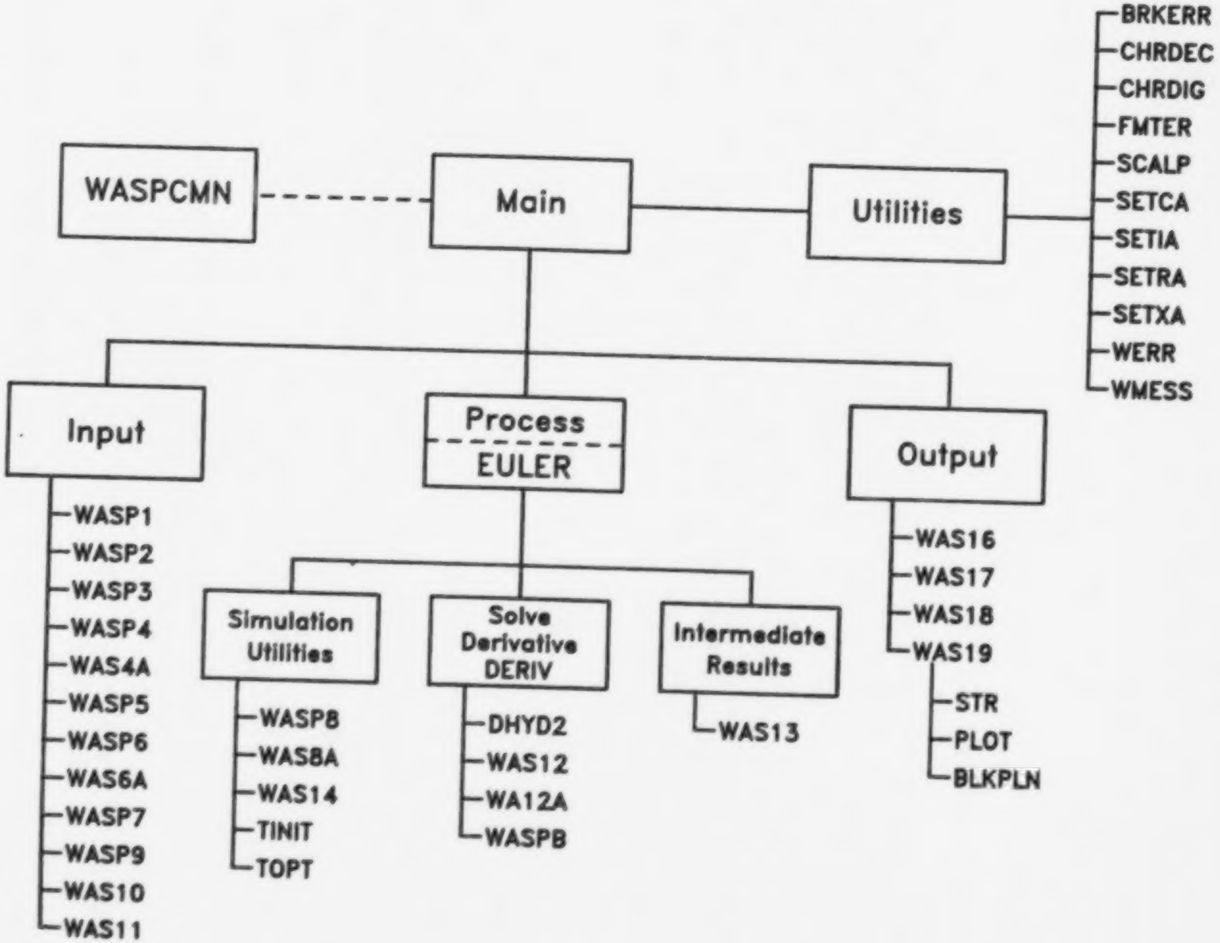

WASPCMN
Main
Utilities
BRKERR
CHRDEC
CHRDIG
FMTER
SCALP
SETCA
SETIA
SETRA
SETXA
WERR
WMESS
Input
WASP1
WASP2
WASP3
WASP4
WAS4A
WASP5
WASP6
WAS6A
WASP7
WASP9
WAS10
WAS11
Process
EULER
Simulation Utilities
WASP8
WAS8A
WAS14
TINIT
TOPT
Solve Derivative DERIV
DHYD2
WAS12
WA12A
WASPB
Intermediate Results
WAS13
Output
WAS16
WAS17
WAS18
WAS19
STR
PLOT
BLKPLN

Figure 54. WASP program structure.

```
C ++++++++++ FILE WSPCMN.F4P ++++++++++
C
C***********************************************************************
C                       COMMON BLOCK FOR THE
C                      IBM PC VERSION OF WASP
C************************************************ LAST REVISED 12/20/85
C
C     ASSIGN SY=SYSTEMS, SG=SEGMENTS, CS=CONSTANTS, PR=PARAMETERS
C            BC=BOUNDARY CONC'S, WK=LOADS, TF=TIME FUNCTIONS
C            MP=MAX PRINT REC'S, MD=MXDMP, MB=MAX NO. BREAKS OR TF'S
C***********************************************************************
      INTEGER SY, SG, S2, CX, PR, BC, WK, TF, MP,MB,MD,MDU,MB1
      INTEGER MV,M30,M50,M70,M72,M73,M75
      PARAMETER (SY=2, SG=80, S2=SG+SG, CX=85, PR=21, BC=20, WK=10,
     . TF=6, MP=50, MB=40, MD=8, MDU=MD*SG, MB1=MB+1, MV=MD*SG*MP,
     . M30=2*BC*SY, M50=2*WK*SY, M70=S2+1, M72=S2+1, M73=2*TF, M75=2*MB)
C
C***********************************************************************
C
      REAL      NVOLT,NRT,NQT,NBCT,NWKT,NFUNT,NFT,NTB,NTW
      REAL      MVOL,MR,MQ,MBC,MWK,MFUNC,NPSWK
      INTEGER   IN,HYDRO,AUX,FRQ,RESTRT,SCRN,OUT,SYSBY,RBY,QBY
      LOGICAL*4 ANCHOR
      REAL*8    AIMASS,AOMASS,RIMASS,ROMASS,XLMASS,XKMASS,XBMASS,XMASS0
      REAL*8    CD
C***********************************************************************
C          INTEGERS
      COMMON /INTGR/ IN,ICRD,OUT,AUX,RESTRT,HYDRO,SCRN,
     .         NOSYS,NOSEG,ISYS,ISEG,ISIM,LISTG,LISTC,NPRINT,
     .         INITB,IPRNT,IDUMP(8,2),IDISK,IREC,MXDMP,IDFRC(19),
     .         NBCPSY,NWKPSY,SYSBY(SY),RBY(SY),QBY(SY),NEGSLN,
     .         IR(S2),JR(S2),IQ(S2),JQ(S2),IBC(SY,BC),IWK(SY,WK),
     .         IVOPT,NOV,IROPT,NOR,IQOPT,NOQ,IBCOP(SY),NOBC(SY),
     .         IWKOP(SY),NOWK(SY),NOPAM,NCONS,NFUNC,
     .         ITIMR,ITIMV,ITIMQ,ITIMF(TF),ITIMB(SY,BC),ITIMW(SY,WK),
     .         ITCHCK,MXITER,INPERR,FRQ
C          REALS
      COMMON /REAL/ ANCHOR,TIME,DT,TZERO,SCALT,TEND,PRNT,OMEGA,
     .         CD(SY,SG),C(SY,SG),CMAX(20),CMIN(SY),
     .         PARAM(SG,PR),CONST(CX),
     .         BVOL(SG),BR(S2),BQ(S2),BBC(SY,BC),BWK(SY,WK),BFUNC(TF),
     .         MVOL(SG),MR(S2),MQ(S2),MBC(SY,BC),MWK(SY,WK),MFUNC(TF),
     .         NVOLT,NRT, NQT, NTF, NBCT(SY,BC),NWKT(SY,WK),NFUNT(TF),
     .         NTB(TF),NTW(TF)
C          LABELLED
      COMMON   /PDP/ MXSYS,MXSEG
      COMMON   /MASS/ AIMASS,AOMASS,RIMASS,ROMASS,XLMASS,XKMASS,XBMASS,
     •                XMASS0
      COMMON   /CPRINT/  PRINT(20),TPRNT(20),ADFAC,TPRINT
      COMMON   /DAYIND/  DAY,LDAY,NDAY,NEWDAY,DQTIME,DRTIME,DWKTIM
      COMMON   /NPSCOM/  NPSWK(SY,WK),INPS(WK),NWKS,NOWKS,LOPT
C          INTERMEDIATE FILES
      COMMON   /SCRTCH/ FILE30(MB,M30),FILE50(MB,M50),FILE70(MB,M70),
     •                   FILE72(MB,M72),FILE73(MB,M73),FILE75(M75,1),
     •                   FILE80(SY,20),NBRK30(BC),NBRK50(WK),NBRK70(1),
     •                   NBRK72(1),NBRK73(TF),NBRK75(1)
      COMMON   /DUMP/    DTIME(MP),DVAR(MV,SY),DVOL(MP,SG)
C
C*******************************************************************
C
C ++++++++++ END OF FILE WSPCMN.F4P ++++++++++
C
```

```
C***********************************************************************
C                            EU03WSP3.CMN
C                       IBM 3033 VERSION OF WASP
C*********************************************** LAST REVISED 03/06/85
C
C     ASSIGN SY=SYSTEMS, SG=SEGMENTS, CS=CONSTANTS, PR=PARAMETERS
C            BC=BOUNDARY CONC'S, WK=LOADS, TF=TIME FUNCTIONS
C            MP=MAX PRINT REC'S, MD=MXDMP, MB=MAX NO. BREAKS OR TF'S
C***********************************************************************
      INTEGER SY, SG, S2, CX, PR, BC, WK, TF, MP,MB,MD,MDU,MB1
      INTEGER MV,M30,M50,M70,M72,M73,M75
      PARAMETER (SY=8, SG=30, S2=SG+SG, CX=75, PR=15, BC=40, WK=20,
     . TF=14, MP=50, MB=50, MD=4, MDU=MD*SG, MB1=MB+1, MV=MD*SG*MP,
     . M30=2*BC*SY, M50=2*WK*SY, M70=S2+1, M72=S2+1, M73=2*TF, M75=2*MB)
C
C      PARAMETER (SY=8, SG=50, S2=SG+SG, CX=75, PR=15, BC=50, WK=50,
C     . TF=14, MP=50, MB=60, MD=4, MDU=MD*SG, MB1=MB+1, MV=MD*SG*MP,
C     . M30=2*BC*SY, M50=2*WK*SY, M70=S2+1, M72=S2+1, M73=2*TF, M75=2*MB)
C***********************************************************************
      REAL      NVOLT,NRT,NQT,NBCT,NWKT,NFUNT,NFT,NTB,NTW
      REAL      MVOL,MR,MQ,MBC,MWK,MFUNC,NPSWK
      INTEGER   IN,HYDRO,AUX,FRQ,RESTRT,SCRN,OUT,SYSBY,RBY,QBY
      LOGICAL*4 ANCHOR
      REAL*8    AIMASS,AOMASS,RIMASS,ROMASS,XLMASS,XKMASS,XBMASS,XMASSO
      REAL*8    CD
C***********************************************************************
C         INTEGERS
      COMMON /INTGR/ IN,ICRD,OUT,AUX,RESTRT,HYDRO,SCRN,
     .         NOSYS,NOSEG,ISYS,ISEG,ISIM,LISTG,LISTC,NPRINT,
     .         INITB,IPRNT,IDUMP(8,2),IDISK,IREC,MXDMP,IDFRC(19),
     .         NBCPSY,NWKPSY,SYSBY(SY),RBY(SY),QBY(SY),NEGSLN,
     .         IR(S2),JR(S2),IQ(S2),JQ(S2),IBC(SY,BC),IWK(SY,WK),
     .         IVOPT,NOV,IROPT,NOR,IQOPT,NOQ,IBCOP(SY),NOBC(SY),
     .         IWKOP(SY),NOWK(SY),NOPAM,NCONS,NFUNC,
     .         ITIMR,ITIMV,ITIMQ,ITIMF(TF),ITIMB(SY,BC),ITIMW(SY,WK),
     .         ITCHCX,MXITER,INPERR,FRQ
C         REALS
      COMMON /REAL/ ANCHOR,TIME,DT,TZERO,SCALT,TEND,PRNT,OMEGA,
     .         CD(SY,SG),C(SY,SG),CMAX(20),CMIN(SY),
     .         PARAM(SG,PR),CONST(CX),
     .         BVOL(SG),BR(S2),BQ(S2),BBC(SY,BC),BWK(SY,WK),BFUNC(TF),
     .         MVOL(SG),MR(S2),MQ(S2),MBC(SY,BC),MWK(SY,WK),MFUNC(TF),
     .         NVOLT,NRT, NQT, NTF, NBCT(SY,BC),NWKT(SY,WK),NFUNT(TF),
     .         NTB(TF),NTW(TF)
C         LABELLED
      COMMON   /PDP/ MXSYS,MXSEG
      COMMON   /MASS/ AIMASS,AOMASS,RIMASS,ROMASS,XLMASS,XKMASS,XBMASS,
     *                XMASSO
      COMMON   /CPRINT/  PRINT(20),TPRNT(20),ADFAC,TPRINT
      COMMON   /DAYIND/  DAY,LDAY,NDAY,NEWDAY,DQTIME,DRTIME,DWKTIM
      COMMON   /NPSCOM/  NPSWK(SY,WK),INPS(WK),NWKS,NOWKS,LOPT
C          INTERMEDIATE FILES
      COMMON   /SCRTCH/ FILE30(MB,M30),FILE50(MB,M50),FILE70(MB,M70),
     *                  FILE72(MB,M72),FILE73(MB,M73),FILE75(M75,1),
     *                  FILE80(SY,20),NBRK30(BC),NBRK50(WK),NBRK70(1),
     *                  NBRK72(1),NBRK73(TF),NBRK75(1)
      COMMON   /DUMP/    DTIME(MP),DVAR(MV,SY),DVOL(MP,SG)
C
C***********************************************************************
C
```

```
C--------------------------------------------------- TOXIWSPB.COM, 1/28/85
      REAL KAHL,KNHL,KBHL,KOXL,KBACWL,KBACSL,MWTG
      REAL KAHG, KNHG,KBHG,KOXG,KBACWG,KBACSG,K02G,K02L,K20
      REAL INDEXW,INDEXS,KOC,KOW,KP,KB, KVOG,TKEL,JL,IL
      REAL LATG,KDPG,KDPL,LIGHTN
C
      DIMENSION EBHG(3,1),ENHG(3,1),EAHG(3,1),QUANTG(3,1),
     .    KAHG(3,1),KBHG(3,1),KNHG(3,1),EOXG(3,1),KOXG(3,1),KBACWG(3,1),
     .    KBACSG(3,1),QTBAWG(3,1),QTBASG(3,1),TEMPM(SG),DEPTHG(SG),
     .    VELOC(SG),ALPHA(3),BIOTMG(SG),K02G(SG),PHG(SG),WS(SG),
     .    OXRADG(SG),WINDG(SG),TYPEE(SG),TOTKG(SG),ACBACG(SG)
      DIMENSION POHG(SG),OCS(SG), BACTOG(SG),BIOMAS(SG),CMPETG(SG)
      SIMENSION DISPV(SG),KP(SG),PCTWA)SG),FRW(SG),DSPSED(SG)
      DIMENSION VVOL(SG),BVOLO(SG),RVOL(SG),BMASS(SG),VOLKG(SG)
C
C             CONSTANTS
C
C          HYDROLYSIS
      EQUIVALENCE
     .    (CONST(1),EBHG(1,1)),     (CONST(4),ENHG(1,1)),
     .    (CONST(7),EAHG(1,1)),     (CONST(10),KAHG(1,1)),
     .    (CONST(13),KBHG(1,1)),    (CONST(16),KNHG(1,1))
C
C          OXIDATION
      EQUIVALENCE
     .    (CONST(25),KBACWG(1,1)), (CONST(28),QTBAWG(1,1)),
     .    (CONST(31),KBACSG(1,1)), (CONST(34),QTBASG(1,1))
C
C          PARTITIONING
       EQUIVALENCE (CONST(37),KOC), (CONST(38),KOW),(CONST(39),OCB),
     .    (CONST(40),ALPHA(1))
C
C          VOLATILIZATION
      EQUIVALENCE
     .    (CONST(43),MWTG),(CONST(44),HENRYG),(CONST(45),VAPRG),
     .    (CONST(46),KVOG),(CONST(47),SOLG),(CONST(48),ESOLG),
     .    (CONST(49),EVPRG),(CONST(50),EHENG),(CONST(51),WIND),
     .    (CONST(52),K02L),(CONST(53),DUMMY6)
C
C          PHOTOLYSIS
```

```
       EQUIVALENCE (CONST(54),KDPG),
     .     (CONST(55),RFLATG),(CONST(56),CLOUDG),(CONST(57),LATG),
     .     (CONST(58),DFACG),(CONST(59),QUANTG(1,1))
C
C          SPECIAL PRINT OPTIONS
      EQUIVALENCE (CONST(62),XJTR),(CONST(63),CTRIG),(CONST(64),DTOPT),
     .     (CONST(65),TDINT)
C
C          INTERNALLY SAVED CONSTANTS
      EQUIVALENCE (CONST(67),BURY),(CONST(68),KDPL),
     .     (CONST(69,KB),(CONST(70),TEMPN),(CONST(71),TKEL),
     .     (CONST(72),PNEXT(,(CONST(73),TCOUNT),
     .     (CONST(74),TMARK),(CONST(75),XJSTR)
      EQUIVALENCE (CONST(76),PH),(CONST(77),POH),(CONST(78),LIGHTN),
     .     (CONST(79),INDEXW),(CONST(80),INDEXS),(CONST981),BOTLIT),
C    .     (CONST(82),TIMCHK),(CONST(83),MOQS),(CONST(84),NOWKS),
     .     (CONST(85),TMASS)
C
C              PARAMETERS
C
      EQUIVALENCE (PARAM(1,1),TEMPM(1)),(PARAM(1,2),DEPTHG(1)),
     .      (PARAM(1,3),VELOC(1)),(PARAM(1,4),WINDG(1)),(PARAM(1,5),
     .       TYPEE(1)),(PARAM(1,6),BACTOG(1)),(PARAM(1,7),ACBACG(1)),
     .      (PARAM(1,8),BIOMASS(1)),(PARAM(1,9),BIOTMG(1)),
     .      (PARAM(1,10),POHG(1)),(PARAM(1,11),OXRADG(1)),
      EQUIVALENCE
     .      (PARAM(1,12),OCS(1)),(PARAM(1,13),PCTWA(1)),
     .      (PARAM(1,14),DSPSED(1)),(PARAM(1,15),PHG(1)),
     .      (PARAM(1,17),CMPETG(1)),(PARAM(1,16),WS(1)),
     .      (PARAM(1,18),TOTKG(1)),(PARAM(1,19),DISPV(1)),
C
      EQUIVALENCE (PARAM(1,20),VVOL(1)),(VVOL(1),BVOLO(1)),
     .             (VVOL(1),RVOL(1))
      EQUIVALENCE (PARAM(1,14),VOLKG(1)),(PARAM(1,21),BMASS(1))
      EQUIVALENCE (PARAM(1,12),KP(1)),(PARAM(1,13),FRW(1))
      EQUIVALENCE (PARAM(1,3),BO2G(1)),
C
      EQUIVALENCE (IDUMP(1,1),I1),(IDUMP(1,2),J1)
C
C-----------------------------------------------------------------------
```

```
C
C     THIS IS THE INCLUSION 'EUTRO.COM'
C
      COMMON/EUTRO1/
     .        F,      H,      I,     CN,     CS,     C1,     C2,
     .       C3,     C4,     C5,     C6,     C7,     C8,     C9,
     .       GP,     IO,     KA,     KE,             SA,     TN,
     .               DO,     ON,     OP
      COMMON/EUTRO2/
     .      K20,    C10,    C11,    C12,    C13,    C14,    C15,
     .      C16,    C17,    C18,    C19,    DPP,    DP1,    DP2,
     .      DZ1,    DZ2,    DIF,    GPP,    GP1,    GP2,    GZ1,
     .      GZ2,    IAV,    IKE,    ITO,    NH3,    NO3,    SAL,
     .      SKE,    SK9,    SOD,    SR9,    STP,    SUM,    TIN,
     .      TIP,    TON,    TOP,    TSI,    VEL,    VOL,    ZOO,
     .      NO2
      COMMON/EUTRO3/
     .     FLUX,   GIT1,   GIT2,   IBOT,   IMAX,   ITMP,   ITOT,
     .     REAK,   PHYT,   RADJ,   RESP,   SK17,   SK58,   SK68,
     .     SK78,   SK8P,   SR17    SR5P,   SR53,   SR54,   SR6P,
     .     SR63,   SR64,   SR7P,   SR73,   SR74,   SR8P,   SR83,
     .     SR84,   TEMP,   FLOW,   WIND,   UBOD,   OPO4,   CBOD,
     .     BBOD,   BOD5,   PSED,   EXCH
      COMMON/EUTRO4/
     .
     .    PFLUX,  ASSIM,  CCHL1,  SK228,  KOREA,  WINDF,
     .    CCHL2,  BFLUX,  PEXCH,  TFNH4,  SK210,  SR822,  TFPO4,
     .    DOMAX,  CHLA1,  CHLA2,  DEATH,  DELO2,  DERIV,  DODEF,
     .    HGRAZ,  DOMIN,  DTDAY,          DUMMY,  FRPIP,  GRAZP,
                  KESHD,  PTIME,  RATIO,  RESP2,  RNUTR,  SK140
      COMMON/EUTRO5/
     .    SK16P,  SK180,  SK19P,  SK19Z,  SR10P,  SR103,  SR104,
     .    SR11P,  SR113,  SR114,  SR12P,  SR123,  SR124,  SR13P,
     .    SR133,  SR134,  SR15P,  SR18P,  SR183,  SR184,  SR190,
     .    SR80P,  STP20,  SW16A,  TCHLA,  TEMP1,  TEMP2,  TEMP3,
     .    TNLIP,  XEMP1,  XEMP2,  XEMP3,  XEMP4,  ZRESP,  LIMIT
      COMMON/EUTRO6/
     .   CHLA1X, CHLA2X, FXNAVG, GITMAX, GITMX1, GITMX2, GPMDP1,
     .   GPMDP2, GZMDZ1, GZMDZ2, HGRAZE, PNH3G1, PLNH3G2,
     .   RLIGHT, RTOXG1, RTOXG2, SEDSEG, SEDVLS, SK1013, SK1113,
     .   SK1213, SK13P1, SK13P2, SK1314, SK14P1, SK14P2, SK1516,
     .   SK1814, SK1913, SK1918, SR10PU, SR103U, SR11PU, SR113U
      COMMON/EUTRO7/
     .   SR12PU, SR123U, SR13NF, SR13ON  SR13PU, SR133U, SR1413,
     .   SR15PG, SR1615, SR18PU, SR183U, SR19PA, SR19PB, SR5PUN,
     .   SR53UN, SR6PUN, SR63UN, SR7PUN, SR73UN, SR8PUN, SR83UN,
      •   TCHLAX, TZOOPL, XDUM89, XDUM95, XEMPRC, ZGRAZE, ZRESP1,
      •   ZRESP2, BOTBOD, DEPTHM, WINDSG, VELSGM, TRANDP,
      •   TEMPSG, SR1821, SK2118, SK1921, PSEDIM,
      •   BSEDIM, AVDEPE, AVVELE, CFOREA, EXPRED, EXPREV
C
C
       LOGICAL SEDSEG, SW16A
       REAL       AVDEPE,AVVELE,CFOREA,
      •           EXPRED,EXPREV,KOREA,REAK,
      •           DIF,TRANDP,WINDF
       REAL   NH3,NO3,LIMIT,No2,K2013C,K2013T,NUTLIM,K1320C,K1320T
      •   ,K2014C,K2014T
       REAL   K1C,K1T,LGHTSW,IS1,KMNG1,KMPG1,KMSI,K1RC,K1RT,K1D,KMPHYT
      •   ,NCRB,K2C,K2T,IS2,KMNG2,KMPG2,K2RC,K2RT,K2D,KMCG,KMAZP1,K3RC
      •   ,K3RT,K3D,K4RC,K4RT,K4D,K58C,K58T,K68C,K68T,K78C,K78T,K1013C
      •   ,K1013T,K1113C,K1113T,K1213C,K1213T,K1314C,K1314T,KNIT
      •   ,K140C,K140T,KNO3,K1516C,K1516T,KDC,KDT,KBOD,ITOT,NITFIX
      •   ,KCLTX1,KCLTX2
       REAL   KPZDC,KPZDT,KOPDC,KOPDT,KONDC,KONDT,KUSDC,KUSDT,KDSC,KDST
       REAL   KE(5),TEMP(4),DEPTH(SG),TYPEE(SG),BOTSG(SG),VELSG(SG)
      •   ,TMPSG(SG),KESG(SG),RLGHTS(SG,2),EDIF(SG),SOD1D(SG),FPIPWC(SG)
      •   ,FNH4(SG),FPO4(SG)
       REAL   KESHD,IAV,IMAX,IO,KA,K20
       REAL BCT(MP)
C
       EQUIVALENCE   (CONST(1),K1C) , (CONST(2),K1T) , (CONST(3),LGHTSW)
      •   , (CONST(4),PHIMX ) , (CONST(5),XKC   ) , (CONST(6),CCHL  )
      •   , (CONST(7),IS1    ) , (CONST(8),KMNG1 ) , (CONST(9),KMPG1 )
       EQUIVALENCE
      •     (CONST(10),K1RC  ) , (CONST(11),K1RT  ) , (CONST(12),K1D   )
      •   , (CONST(13),KMPHYT) , (CONST(14),PCRB  ) , (CONST(15),NCRB  )
      •   , (CONST(16),OCRB  ) , (CONST(17),NUTLIM) , (CONST(18),FPIPWX)
      •   , (CONST(19),FPIPSL) , (CONST(20),FSOP  ) , (CONST(21),FSIP  )
      •   , (CONST(22),FSON  ) , (CONST(23),K58C  ) , (CONST(24),K58T  )
      •   , (CONST(25),K1013C) , (CONST(26),K1013T) , (CONST(27),K1320C)
       EQUIVALENCE
      •     (CONST(28),K1320T) , (CONST(29),K2014C) , (CONST(30),K2014T)
      •   , (CONST(31),KNIT  ) , (CONST(32),KBOD  ) , (CONST(33),KDC   )
      •   , (CONST(34),KDT   ) , (CONST(35),SVP1  ) , (CONST(36),SVPP  )
      •   , (CONST(37),SVPN  ) , (CONST(38),SVBOD ) , (CONST(39),SEDVEL)
      •   , (CONST(40),SCOUR ) , (CONST(41),KPZDC ) , (CONST(42),KPZDT )
      •   , (CONST(43),KOPDC ) , (CONST(44),KOPDT ) , (CONST(45),KONDC )
      •   , (CONST(46),KONDT ) , (CONST(47),KDSC  ) , (CONST(48),KDST  )
      EQUIVALENCE
     .     (CONST(49),KMCG  ) , (CONST(50),CGC    ) , (CONST(51),CGT    )
     .   , (CONST(52),AZP1  ) , (CONST(53),KMAZP1) , (CONST(54),K3RC   )
     .   , (CONST(55),K3RT  ) , (CONST(56),K3D    ) , (CONST(57),SVZ1   )
      EQUIVALENCE
     .    (CONST(59),PI), (CONST(74),T16A) , (CONST(75),TIMCHK)
      EQUIVALENCE
     .   (PARAM(1,1),DEPTH(1)) , (PARAM(1,2),TYPEE(1))
     .  ,(PARAM(1,3),BOTSG(1)) , (PARAM(1,4),VELSG(1))
     .  ,(PARAM(1,5),TMPSG(1)) , (PARAM(1,7),KESG(1))
     .  ,(PARAM(1,9),EDIF(1))  , (PARAM(1,10),SOD1D(1))
      EQUIVALENCE                (PARAM(1,11),FPIPWC(1)),
     .   (PARAM(1,12),FNH4(1))   , (PARAM(1,13),FPO4(1)),
     .   (PARAM(1,14),RLGHTS)1,1)) , (PARAM(1,15),RLGHTS(1,2))
C        NPSWK COVERED PARAM (1,16) THROUGH PARAM(SG,20)
C
```

3.3.4.3 Subroutine Descriptions--

WASP3 is a modular program. Its many subroutines can be grouped into the functional categories of "input," "process," "output," and "utility," as in Figure 54. Data are shared among the subroutines primarily through the WASP COMMON.

MAIN

The WASP3 main program is the control module. It assigns input and output unit numbers, and operates the calling sequence for the input, simulation, and output subroutines.

Input Subroutines

WASP1

WASP1 opens the input and output units, then reads Data Group A for model identification and system bypass options. Information is printed and values and arrays are initialized.

WASP2

WASP2 reads Data Group B for either bulk exchanges or sets of dispersion coefficients, cross-sectional areas, and characteristic lengths. The latter are converted to bulk exchanges, and information is stored in memory and printed.

WASP3

WASP3 reads Data Group C for volumes. If indicated, volumes are read from restart file "ICRD." Information is stored in memory and printed.

WASP4

WASP4 reads Data Group D for advective flows, which are converted to internal units of million cubic feet per day. Information is stored in memory and printed. If indicated, WAS4A is called to read flows from a hydrodynamic file created by DYNHYD3.

WAS4A

If indicated, WAS4A opens the hydrodynamic file "SUMRY2.OUT" created by DYNHYD3, and reads some basic hydrodynamic network information in either a formatted or unformatted mode. WAS4A then reads the junction to segment correspondence, sets the WASP time step, and prints information.

WASP5

WASP5 reads Data Group E for boundary concentrations for each model system. Information is stored in memory and printed.

WASP6

WASP6 reads Data Group F for waste loads for each model system. Information is stored in memory and printed.

WAS6A

If indicated, WAS6A opens the unformatted loading file "NPS.DAT" created by a runoff model and stored in the sequence illustrated in Table 22. The runoff day corresponding with the initial WASP simulation day is read. Input segment numbers corresponding to each runoff load are read. Actual runoff loads from the file are printed as specified. Finally, the file is positioned properly to begin the WASP simulation.

TABLE 22. CONTENTS OF "NPS.DAT"

Record Number	Contents of Record
1	NWKS, MDUM, MDUM, MDUM
2	((NPSWK(I,J),I=1,NOSYS),J=1,NWKS)
3	((NPSWK(I,J),I=1,NOSYS),J=1,NWKS)
.	
.	
.	
N+1	((NPSWK(I,J),I=1,NOSYS),J=1,NWKS)

Variable	Type	Definition
NWKS	I*4	The number of runoff loads
MDUM	I*4	Dummy variable, not used
NPSWK	R*4	Runoff loads, averaged over day, in lb/day
NOSYS	I*4	Number of water quality variables (or systems)
I	I*4	Water quality variable counter
J	I*4	Runoff load counter
N	--	Number of days for which loads are available

WASP7

WASP7 reads Data Group G for parameters for each segment. It then reads Data Group H for constants. Finally, it reads a specified number of kinetic time functions. Information is stored in memory and printed.

WASP9

WASP9 reads Data Group J for initial concentrations in all segments for each model system. Versions 2 and 3 of WASP expect the first data record to be a descriptive "header" card. If not, WASP9 uses functions CHRDEC and CHRDIG to convert the line to input concentrations expected by the original WASP. If indicated, initial concentrations are read from restart file "ICRD." Information is stored in memory and printed. WASP9 finally reads Data Group K for maximum and minimum concentrations for each model system.

WAS10

WAS10 reads Data Group L for constant or variable print intervals. Next, either eight system-segment pairs are read for intermediate printout during the simulation, or a model system is read for a global mass balance check. Information is stored and printed.

WAS11

WAS11 reads Data Group M for integration control information, including the starting and ending time for the simulation, a series of time step sizes, the negative solution option, and the advection factor. Information is stored in memory and printed.

Process Subroutines

Once input data groups A-M are read, control is passed to EULER to perform the simulation.

EULER

EULER is the heart of the simulation, stepping through time performing a first-order EULER integration. First, counters and time functions are initialized to TZERO with help from subroutine TINIT. Initial printouts are set up with a call to WAS13, then initial mass derivatives are computed with a call to DERIV. A fatal input error condition is checked for, then the integration proceeds, time step by time step.

For each time step, EULER loops through each system and segment, computing the new mass as follows:

new mass = old mass + mass derivative . time step

Each new concentration is set to the new mass divided by the new volume, and the mass derivative is reset to zero. If the negative solution option is "0," any negative concentrations are replaced by one-half of the old mass divided by the new volume. Next, EULER increments the time and adjusts the new day counter if necessary. If it is the proper time, EULER calls WAS13 to produce intermediate printouts and trigger storage of all display variables (by returning IDISK = 1). New mass derivatives are obtained with a call to DERIV. Volumes are stored if IDISK = 1. The final task for each time step is to check for a new time step and for the end of the simulation. New time steps are periodically set by calling WAS14.

When the final time for the simulation is detected, EULER triggers a final storage of display variables, then stores final volumes and concentrations in file "RESTRT." Control is then passed back to MAIN.

DERIV

DERIV is called by EULER to calculate mass derivatives. It first checks and obtains new flows and volumes from a hydrodynamic file by calling DHYD1 or DHYD2. It then obtains the kinetic derivative by calling WASPB. Finally, it obtains the transport and loading derivatives by calling WAS12.

DHYD1 and DHYD2

One of these subroutines may be called by DERIV to obtain new hydrodynamic information from the hydrodynamic file "SUMRY2.OUT," created by DYNHYD3. These subroutines are equivalent, except that DHYD1 reads an unformatted file while DHYD2 reads a formatted file.

For the first time step, DHYDx reads the basic hydrogeometry and initializes its arrays. Hydrodynamic junction to water quality segment correspondence is established, and flow directions are fixed. Upstream and seaward boundaries are set up, and boundary concentrations are located for each. The hydrodynamic file is positioned properly in time, and flows for the first time step are printed.

For each time step throughout the simulation, DHYDx is called and reads new flows and volumes from SUMRY2.OUT. These are scaled and converted to internal WASP3 units. New boundary flows are set up. If the end of the hydrodynamic file is properly detected, it is reset to its beginning point, and the simulation proceeds. If the file end is improperly detected in the middle of a read, the simulation is aborted.

WAS12

WAS12 is called by DERIV to obtain the transport and loading derivatives. Upon entry to WAS12, only the kinetic portion of the mass balance derivative has been evaluated by WASPB. WAS12 calculates the mass derivatives due to advective flow, dispersive exchange, point source waste loading, and runoff loading, and adds them to the kinetic derivative. WAS12 goes through the following steps:

a. Using the IQ and JQ vectors as drivers, WAS12 computes advective transport. Variable flows are updated by calling WASP8 if necessary, and volumes are adjusted for continuity. For each system, variable boundary concentrations are updated by calling WAS8A if necessary. For each flow, Q, proper upstream and downstream concentrations are assigned by calling WA12A. The advected concentration CSTAR is determined, and mass derivatives for the downstream and upstream segments are adjusted by ± Q.CSTAR.

b. Using the IR and JR vectors as drivers, WAS12 computes dispersive transport. Variable exchanges are updated by calling WASP8 if necessary. For each system and each exchange flow, R, proper upstream and downstream concentrations C_2 and C_1 are assigned by calling WA12A. Mass derivatives for the downstream and upstream segments are adjusted by $\pm R \cdot (C_2-C_1)$.

c. Using the IWK vector as a driver, WAS12 computes point source loading. For each system, variable loadings are updated by calling WAS8A if necessary. For each load L (in lb/day), the mass derivative for the affected segment is adjusted by + L/62.4.

d. Using the INPS vector as a driver, WAS12 computes diffuse source loading if appropriate. New loads are read from file NPS.DAT at the beginning of each new day. For each load L' (in lb/day), the mass derivative for the affected segment is adjusted by + L'/62.4.

WA12A

WA12A is called by WAS12 to determine the proper upstream and downstream concentrations C_2 and C_1 for advective flow from segment JQ to segment IQ or dispersive exchange between segments JR and IR. For flows or exchanges with a downstream boundary, the proper boundary concentration is located for C_1. For flows or exchanges with an upstream boundary, the proper boundary concentration is located for C_2.

WASPB

WASPB is the user-specified water quality subroutine that calculates the kinetic mass derivative and stores the proper display variables for later printout. WASPLB may call several other subroutines. These are discussed below for eutrophication and toxic chemical subroutines.

WASP8

WASP8 is called by WAS12 to update the piecewise linear functions of time, if any, for exchange coefficients, advective flows, and kinetic time functions. This means computing new slopes and intercepts, and setting a variable to indicate the next simulation time that the functions are to be updated. The following convention is used for the i^{th} update.

$$\text{slope} = \frac{f(t)_{i+1} - f(t)_i}{t_{i+1} - t_i}$$

$$\text{intercept} = f(t)_{i+1}$$

$$\text{next update time} = t_{i+1}$$

WAS8A

WAS8A is used to update the piecewise linear functions of time, if any, for boundary conditions and forcing functions. This means computing new slopes and intercepts for any system or state variable that requires an update, and setting a variable to indicate the next simulation time that the piecewise linear functions are to be updated. The same conventions used in WASP8 are used in WAS8A for computing slopes and intercepts.

WAS13

WAS13 is called every print interval by EULER to print intermediate concentrations or mass checks on a designated constituent. At this time, the solution stability is checked by comparing the maximum concentrations specified by the user with calculated concentrations. If any concentrations exceed the maximum, the simulation is aborted.

WAS14

WAS14 is called by EULER to adjust the integration step size (time step) as specified by the user in Data Group M.

TINIT

TINIT is called by EULER at the beginning of the simulation to adjust time functions to the initial time TZERO. TINIT checks and adjusts time functions for exchanges, flows, kinetic time functions, boundary concentrations, and loads.

TOPT

TOPT can be called by the user WASPB subroutine to maximize the time step subject to the flow and dispersion stability constraints. This should reduce numerical dispersion, but is not unconditionally stable. The time step calculated by TOPT is 0.5 days will fall between 0.01 and 0.5 days.

Output Subroutines

Once the simulation is complete, control is passed to the output subroutines to print tables, time plots, and spatial plots.

WAS16

WAS16 reads Data Group N system by system to determine what tables the user wants printed. Designated state variable concentrations and display variables are retrieved from memory and printed at all print intervals covered by the simulation. There is no limit to the number of tables that can be specified. The total mass in each system is calculated and printed at each print interval following the tables.

WAS17

WAS17 reads Data Group O system by system to determine what time plots the user wants printed. Designated state variable concentrations and display variables are retrieved from memory and plotted at all print intervals covered by the simulation. There is no limit to the number of time plots that can be specified.

WAS19 (including STR, PLOT, BLKPLN)

WAS19 reads Data Group P to determine what spatial plots the user wants printed. Designated state variable concentrations and display variables are retrieved from memory and plotted for all segments at designated times. Observed data can be read and included on the plots. There is no limit to the number of spatial plots that can be specified.

FREQ (including ORDER)

FREQ is called if the switch ISTAT is activated in the users WASPB subroutine. The unformatted file "FREQ.TMP" must be produced by the WASPB subroutine during the simulation. A set of three records should have been stored at regular intervals throughout the simulation, as specified in Table 23. FREQ reads the detailed concentration time history for the two designated segments, computes and prints descriptive statistics, then prepares and prints cumulative probability tables.

Utility Subroutines

Several utility subroutines can be called to help perform routine tasks.

TABLE 23. CONTENTS OF "FREQ.TMP"

Record Number	Contents of Record
1	TZERO, TIME, ICOUNT, JTR, JSTR
2	ICOUNT, TIME, (CC1(K), K=1,4)
3	ICOUNT, TIME, (CC2(K), K=1,4)
.	
.	
.	
.	

Variable	Type	Definition
TZERO	R*4	Initial simulation time, days
TIME	R*4	Simulation time for this group of records, days
ICOUNT	I*4	The sequence number for this group of records
JTR	I*4	The segment number for the first set of concentrations
JSTR	I*4	The segment number for the second set of concentrations
CC1(K)	R*4	Concentrations of four constituents in segment JTR at this simulation time
CC2(K)	R*4	Concentrations of four constituents in segment JSTR at this simulation time.

BRKERR

BRKERR prints an error message to output file and screen concerning the number of data points in a time function; the simulation is aborted.

CHRDEC

CHRDEC is a real function that converts a character string to its real equivalent.

CHRDIG

CHRDIG is an integer function that converts a character to its integer equivalent.

FMTER

FMTER prints an error message to output file and screen concerning input data formats; the simulation is aborted.

SCALP

SCALP multiplies a real vector by a scale factor.

SETCA

SETCA sets a character array to a specified character value.

SETIA

SETIA sets an integer array to a specified integer value.

SETRA

SETRA sets a real array to a specified real value.

SETXA

SETXA sets a double precision array to a specified double precision value.

WERR

WERR writes error messages for improper segment designations and missing boundary conditions; the simulation is aborted.

WMESS

WMESS prints a message when stability criteria are violated; the simulation is aborted.

Eutrophication Kinetic Subroutines

The WASP3 eutrophication kinetics are calculated through a special WASPB subroutine structure, illustrated in Figure 55. These subroutines combine biological and chemical constants with environmental parameters to determine transformation rates among the eight eutrophication systems (state variables). From these rates and the concentrations passed by WASP, kinetic mass derivatives are calculated and passed back to WASP where they are integrated along with the transport and loading derivatives every time step.

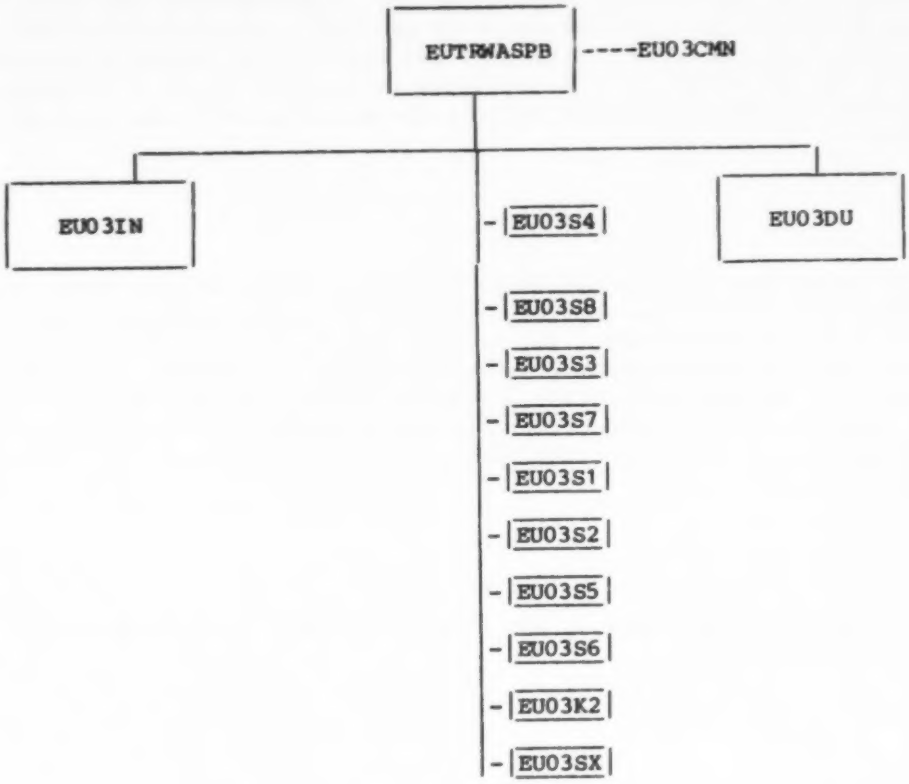


Figure 55. Eutrophication subroutine structure.

WASPB (EUTRWASPB)

EUTRWASPB serves as the main program for the kinetic portion of EUTRWASP, calling other subroutines when appropriate. Initialization is performed during the first time step by calling EU03IN. Kinetic time functions are updated throughout the simulation. For each segment, ambient concentrations and environmental conditions are determined, then mass derivatives are obtained with successive calls to EU03S4, EU03S8, EU03S3, EUO3S7, EUO3S1, EUO3S2, EUO3S5, and EUO3S6. At print intervals, state variable and display variable concentrations are stored by calling EUO3DU. Finally, EUO3SX is called to calculate the exchange of dissolved phases between water column and benthic segments and adjust the derivatives.

EUO3IN

EUO3IN is called during the first time step only to initialize parameters, counters, and functions for the simulation. For the phytoplankton system, initial and boundary concentrations are converted from the input units of ug-Chla/L to the internal units of mg-CRB/L. Sedimentation and scour velocities are converted to ft/day, and water column-benthic exchange coefficients are converted to bulk exchanges in internal units of MCF/day. Finally, benthic fluxes of NH_4 and PO_4 are converted to internal loadings in mg/L . MCF/day.

EUO3S4

EUO3S4 calculates the phytoplankton kinetics, and is called first because it affects all the other systems. For water column segments, the growth rate is first calculated. The maximum growth rate is adjusted for temperature, then reduced according to ambient light conditions using either the Dick Smith or DiToro formulation. Ammonia preference is calculated, then the growth rate is further reduced if nitrogen or phosphorus is in limited supply. Respiration, death, and settling rates are calculated, and, finally, the mass derivative.

EUO3S8

EUO3S8 calculates the sources and sinks of organic phosphorus and computes the mass derivative.

EUO3S3

EUO3S3 calculates the sources and sinks of inorganic phosphorus and computes the mass derivative.

EUO3S7

EUO3S7 calculates the sources and sinks of organic nitrogen and computes the mass derivative.

EUO3S1

EUO3S1 calculates the sources and sinks of ammonia nitrogen and computes the mass derivative.

EUO3S2

EUO3S2 calculates the sources and sinks of nitrite plus nitrate nitrogen and computes the mass derivative.

EUO3S5

EUO3S5 calculates the sources and sinks of carbonaceous biochemical oxygen demand and computes the mass derivative.

EUO3S6

EUO3S6 calculates the sources and sinks of dissolved oxygen and computes the mass derivative. The reaeration rate is obtained for surface water segments by calling EUO3K2.

EUO3K2

EUO3K2 calculates the ambient reaeration rate based on temperature, wind speed, water velocity, and water depth. The current-driven portion of this rate is calculated using the Covar method, which chooses among three formulas based upon velocity and depth. The oxygen saturation level is finally calculated as a function of water temperature.

EUO3DU

EUO3DU is called every print interval to store state variable and display variable concentrations. First the display variables are calculated, then the simulation time is stored in memory. Address counters for the storage arrays are calculated, and four variables are stored in memory for each system.

EUO3SX

EUO3SX calculates the dispersive exchange of dissolved phases between water column and benthic segments, and adjusts the mass derivatives accordingly. If no benthic segments are present, this calculation is skipped. Finally, additional ammonium and phosphate fluxes as specified by the user are added, and derivatives are adjusted.

Toxic Chemical Kinetic Subroutines

The WASP3 toxic chemical kinetics are calculated through a special subroutine structure, illustrated in Figure 56. These subroutines combine chemical and environmental parameters to produce first-order rate constants and, from chemical concentrations passed by WASP, calculate kinetic derivatives. These derivatives are passed back to WASP where they are integrated along with the transport and loading derivatives every time step.

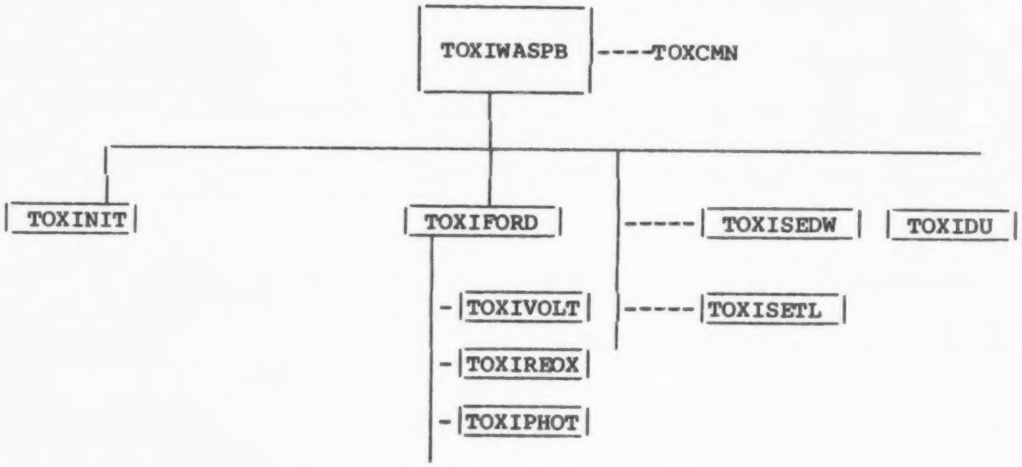


Figure 56. Toxics subroutine structure.

WASPB (TOXIWASPB)

TOXIWASPB serves as the main program for the kinetic portion of TOXIWASP, calling other subroutines when appropriate. Initialization is performed during the first time step by calling TOXINIT. As the simulation progresses, the proper time- and space-variable environmental and chemical characteristics are calculated, then passed to TOXIFORD. Kinetic derivatives are calculated based on first-order rate constants returned from TOXIFORD. These derivatives are then adjusted for settling, erosion, and percolation by calling TOXISETL. Further adjustments in the derivatives due to pore water mixing and sediment-water exchange are calculated by calling TOXISEDW. Variables are periodically dumped to a save file and intermediate parameters and results are printed by calling TOXIDUMP. Finally, the time step is optimized by calling TOPT, if the user chooses.

TOXINIT

TOXINIT is called during the first time step only to initialize parameters and functions for the chemical simulation. The top sediment layer for the special print segment is identified. Effective partition coefficients for each segment are calculated from either the organic carbon or octanol-water partition coefficient, the spatially variable sediment organic carbon fractions, and the target organism organic carbon content. For benthic segments, the units of biomass are adjusted and porosity is calculated. The active bacterial population is calculated for all segments. Initial and reference bed volumes are saved, values are initialized to 0, and CMAX(1) is set to assure the first-order decay assumption. Finally, TOXINIT checks for proper segment alignment, with assigned numbers increasing sequentially from water surface to bottom benthic segments.

TOXIFORD

TOXIFORD, a modification of the EXAMS subroutine FIRORD, calculates total first order chemical transformation rates for each segment as the simulation progresses. The total first-order rate for each segment is the summation of the transformation (including degradation or transfer) rates due to five processes: hydrolysis, oxidation, bacterial degradation, volatilization, and photolysis. These individual rates are calculated from ambient environmental and chemical characteristics passed from TOXIWASPB.

Whenever total rates are to be recalculated during a simulation, TOXIWASPB calls TOXIFORD once for each segment. TOXIFORD first calculates the volatilization transfer rate of dissolved chemical from surface water segments by calling TOXIVOLT. Next, the photolysis rate constant is calculated for water segments by calling TOXIPHOT. Then, for each species of the chemical (dissolved, sediment-sorbed, and biosorbed), first-order transformation rates are calculated for photolysis, hydrolysis, oxidation, and bacterial degradation. Finally these individual rates are summed to give a total first-order chemical disappearance rate, which is passed back to TOXIWASPB.

TOXIVOLT

When called by TOXIFORD, TOXIVOLT computes the volatilization transfer rate constant for a surface water segment using a two-film model of movement of toxicant across the air-water interface. Liquid phase resistance is computed from oxygen reaeration rates modified by the chemical molecular weight. Gas phase resistance is computed from wind speed and Henry's Law constant, which is supplied by the user or calculated from vapor pressure and solubility data. The volatilization rate is computed from the air and water phase resistances and the depth of the surface water segment.

TOXIPHOT

When called by TOXIFORD, TOXIPHOT computes the photolysis transformation rate constant for a water segment. TOXIPHOT accepts a measured (clear day) photolysis rate constant at a specified reference latitude as input data. Next, this rate constant is corrected for the latitude, cloud cover, and light extinction in the water column. The rate is further modified by a time-varying input function to approximate seasonal changes in incident light intensity.

TOXIREOX

TOXIREOX is call by TOXIFORD for surface water segments to calculate reaeration velocities. These are used in TOXIVOLT for calculating volatilization rates. For the first time step only, TOXIREOX calculates average flow-induced reaeration rates by the Covar method (Covar, 1976) using average segment velocities and depths. In subsequent time steps, TOXIREOX calculates time-varying wind-induced reaeration rates. The reaeration rate returned to TOXIFORD is either the flow-induced rate or the wind-induced rate, whichever is larger. TOXIREOX is slightly modified from the HSPF subroutine OXREA.

TOXISETL

TOXISETL is called by TOXIWASPB for each segment and each time step to calculate settling of chemical and suspended sediment from the water column, erosion of chemical in the bed, and percolation of dissolved chemical vertically through the bed. Concentration derivatives are adjusted within TOXISETL. First, settling rates are calculated from spatially variable settling velocities, segment depths, concentrations of sorbed chemical and suspended sediment. Erosion is calculated from spatially variable yearly depletion rates from the bed sediment surface, along with sediment density and sorbed chemical concentration. Bed sediment segments are assumed to maintain their physical characteristics, such as density, porosity, and organic content. Vertical pore water percolation is calculated from spatially variable vertical flow rates, along with porosity and dissolved concentrations. Positive flow is upward, and negative flow is downward. It should be noted that downward percolation will eventually transport the chemical out of the bottom benthic segment.

TOXISEDW

TOXISEDW is called by TOXIWASPB for surface benthic segments each time step to calculate dispersive exchanges of chemical between the bed and the water column. Concentration derivatives are adjusted within TOXISEDW. The two mechanisms are pore water diffusion and local surface sediment equilibration with the water column. Pore water diffusion is calculated from spatially variable diffusion coefficients, surface areas, characteristic mixing lengths, and sediment porosity. Sorption-desorption of chemical between overlying water and the benthic surface is calculated using sediment turnover rates and chemical partition coefficients. Because local equilibrium is assumed, sorption-desorption is controlled by the fraction of underlying sediment brought into contact with the overlying water per unit time. This fraction is related to the pore water diffusion rate by a spatially variable multiplier supplied by the user. For immobile, armored stream reaches, the multiplier may be 0, whereas for reaches vigorously mixed by physical or biological processes, the multiplier may be 1, with high pore water dispersion coefficients as well.

TOXIDUMP

At specified intervals, TOXIWASPB calls TOXIDUMP to prepare or print output from the simulation. Three kinds of output are handled. The first is the standard WASP dump of select variables to a save file at fixed intervals. Eight variables are dumped for "System 1": total chemical concentration (mgc/L_T), dissolved chemical concentration (mgc/L_w), sediment-sorbed chemical concentration (mgc/kgs), biosorbed chemical concentration (ugc/gb), chemical fraction dissolved, chemical fraction sediment-sorbed, chemical mass in segment (kg), and chemical mass lost through volatilization or burial (kg). Eight more variables are dumped for "System 2": total sediment concentration (mgs/L_T), segment depth (ft), the total transformation rate (per day), the photolysis rate, the hydrolysis rate, the biodegradation rate, the oxidation rate, and the volatilization rate (all specific rates in units of per hour).

The second kind of output is event-triggered. When the total chemical concentration exceeds a reference value at a selected segment, total chemical concentrations are printed for every segment every 3 hours until the concentration again falls below the reference.

The third kind of output is the dump of chemical and sediment concentrations at a selected water segment (and its top benthic segment) to a save file every 3 hours. This file is processed by TOXIFREQ after the simulation to yield statistical information, including a cumulative frequency table. Concentrations analyzed include total chemical, dissolved chemical, sediment-sorbed chemical, and biosorbed chemical.

TOXIFREQ (now designated FREQ)

After completion of the simulation, TOXIFREQ processes a file of chemical concentrations at a water and a benthic segment, producing statistical tables. A save file of concentrations written every 3 hours by TOXIDUMP is first ordered by TOXIORDR. Next, the statistics are computed, including minimum, maximum, and mean; various percentiles; standard deviation; skewness; and kurtosis. This table is printed, then a cumulative frequency table is prepared, with concentrations corresponding to ascending even probability values (0.0, 0.02, 0.04,..., 0.98, 1.00). This table is printed, and a plot file is prepared.

3.3.4.4 Overlay Structure--

The size and structure of the WASP program mandated the use of an overlay structure. The overlay procedure facilitated implementation on the personal computer and small mainframe environment.

The purpose of the WASP overlay structure is to insert only the needed portions of the model into memory during simulation. When code is no longer needed, it will be replaced with new required code. Figures 57, 58, and 59 illustrate the overlay structure for WASP3, EUTRWASP, and TOXIWASP, respectively, in a PC environment.

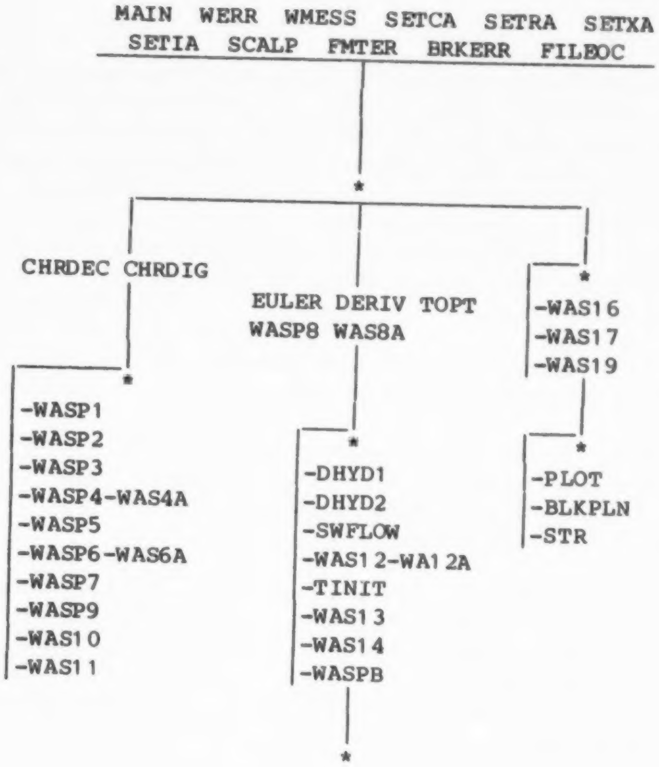

MAIN WERR WMESS SETCA SETRA SETXA
SETIA SCALP FMTER BRKERR FILEOC
*
CHRDEC CHRDIG
*
-WASP1
-WASP2
-WASP3
-WASP4-WAS4A
-WASP5
-WASP6-WAS6A
-WASP7
-WASP9
-WAS10
-WAS11
EULER DERIV TOPT
WASP8 WAS8A
*
-DHYD1
-DHYD2
-SWFLOW
-WAS12-WA12A
-TINIT
-WAS13
-WAS14
-WASPB
*
*
-WAS16
-WAS17
-WAS19
*
-PLOT
-BLKPLN
-STR

Figure 57. PC overlay structure for WASP3.

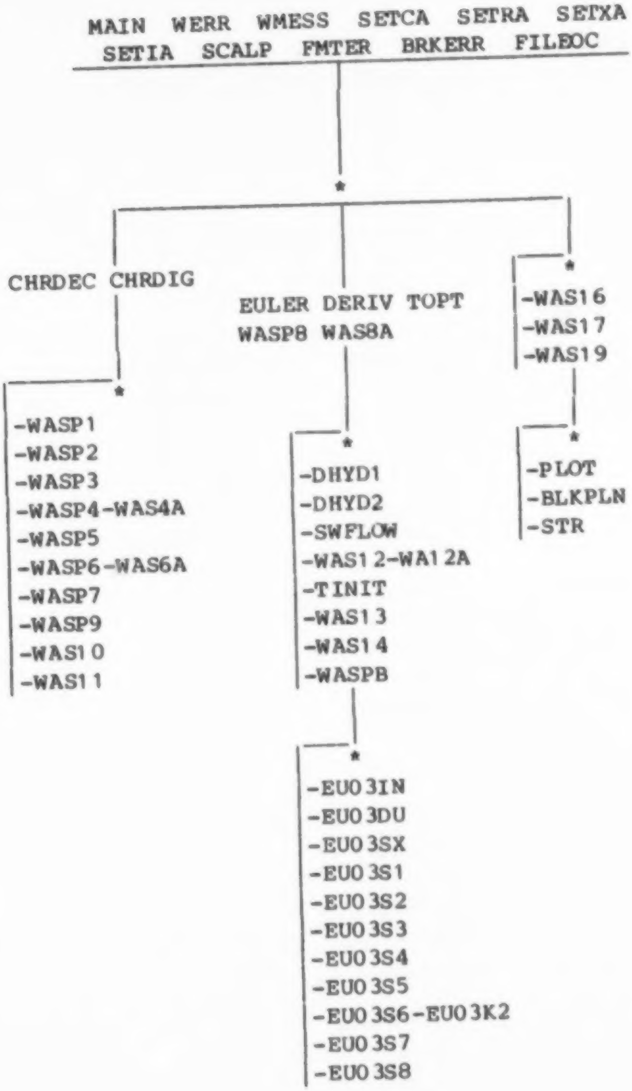

MAIN WERR WMESS SETCA SETRA SETXA
SETIA SCALP FMTER BRKERR FILEOC
*
CHRDEC CHRDIG
*
-WASP1
-WASP2
-WASP3
-WASP4-WAS4A
-WASP5
-WASP6-WAS6A
-WASP7
-WASP9
-WAS10
-WAS11
EULER DERIV TOPT
WASP8 WAS8A
*
-DHYD1
-DHYD2
-SWFLOW
-WAS12-WA12A
-TINIT
-WAS13
-WAS14
-WASPB
*
-EU03IN
-EU03DU
-EU03SX
-EU03S1
-EU03S2
-EU03S3
-EU03S4
-EU03S5
-EU03S6-EU03K2
-EU03S7
-EU03S8
*
-WAS16
-WAS17
-WAS19
*
-PLOT
-BLKPLN
-STR

Figure 58. PC overlay structure for EUTRWASP.

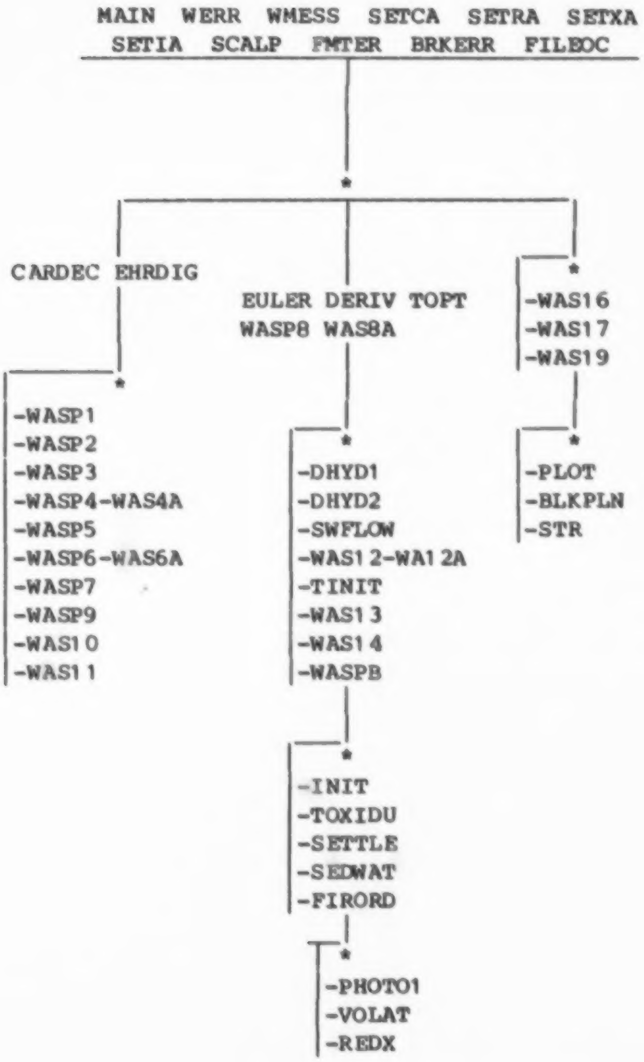

MAIN WERR WMESS SETCA SETRA SETXA
SETIA SCALP FMTER BRKERR FILEOC
CARDEC EHRDIG
-WASP1
-WASP2
-WASP3
-WASP4-WAS4A
-WASP5
-WASP6-WAS6A
-WASP7
-WASP9
-WAS10
-WAS11
EULER DERIV TOPT
WASP8 WAS8A
-DHYD1
-DHYD2
-SWFLOW
-WAS12-WA12A
-TINIT
-WAS13
-WAS14
-WASPB
-INIT
-TOXIDU
-SETTLE
-SEDWAT
-FIRORD
-PHOTO1
-VOLAT
-REDX
-WAS16
-WAS17
-WAS19
-PLOT
-BLKPLN
-STR

Figure 59. PC overlay structure for TOXIWASP.

APPENDIX A

Symbols for Section 1.2

A = cross-sectional area, ft^2.

a_f = frictional acceleration, ft/sec^2.

$a_{g,\ell}$ = gravitational acceleration, ft/sec^2.

A_i = regression coefficients for tidal heights, ft.

A_s = surface area, ft^2.

$a_{w,\ell}$ = wind stress acceleration along axis of channel, ft/sec^2.

b = width, ft.

C_d = drag coefficient (= 0.0026), unitless.

g = acceleration of gravity = 32.2 ft/sec^2.

H = water surface elevation, head, or height above an arbitrary datum, ft.

i = channel or link number, unitless.

ℓ_i = length of channel i, ft.

n = Manning roughness coefficient (usually between 0.01 and 0.10), sec.m$^{-1/3}$.

Q = flow, ft^3/sec.

R = hydraulic radius (approximately equal to the depth), ft.

S = water surface slope, ft/ft.

t = time, hr or sec.

τ_w = the boundary shear stress, lb$_m$/ft-sec^2.

U = velocity along the axis of channel, ft/sec.

$\overline{U}$ = the water velocity (magnitude = U, direction = θ), ft/sec.

U_i = velocity in channel i, ft/sec.

U_i^t = the velocity in channel i at time t, ft/sec.

V_w = water volume, ft^3.

W = the wind speed (relative to the moving water surface) measured at a height of 10 meters above water surface, ft/sec.

$\overline{W}_{obs}$ = the observed wind velocity at a stationary location, ft/sec.

x = distance along axis of channel, ft.

y = tidal elevation above or below the model datum, ft.

y_i = mean depth of channel i, ft.

Δt = the time step, sec.

Δx_i = the channel length, ft.

ρ_a = the density of air, lb_m/ft^3.

ω = tidal frequency, 2π/tidal period, hr^{-1}.

APPENDIX B

Symbols for Section 1.3

A = cross-sectional area, L^2.

C = concentration of the water quality constituent, ML^{-3}.

E_x, E_y, E_z = longitudinal, lateral, and vertical diffusion coefficients, L^2T^{-1}.

L = length units.

ℓ = length of the segment, L.

M = mass units.

Q = volumetric flow = $A \cdot U_x$, L^3T^{-1}.

Q_{ij} = flow, defined as positive when leaving segment j, and negative when entering j, L^3T^{-1}.

R = dispersive flow = $\frac{E.A}{\ell}$, L^3T^{-1}.

S_B = boundary loading rate (including upstream, downstream, benthic, and atmospheric), $ML^{-3}T^{-1}$.

S_K = total kinetic transformation rate; positive is source, negative is sink, $ML^{-3}T^{-1}$.

S_L = direct and diffuse loading rate, $ML^{-3}T^{-1}$.

S_T = total source/sink rate = $S_L + S_B + S_K$, ML^3T^{-1}.

T = time units.

t = time, T.

U_x, U_y, U_z = longitudinal, lateral, and vertical advective velocities, LT^{-1}.

V_j = volume of segment j = $A_j \cdot \ell_j$, L^3.

W_j = point and diffuse loads = $V_j S_{Lj}$, MT^{-1}.

Δt = the time step, typical between 15 minutes and a half day, T.

ν = numerical weighting factor between 0 and 1, unitless.

APPENDIX C

Symbols for Section 1.4

A_{ij} = cross-sectional area between segments i and j, ft^2.

a_{NC} = nitrogen to carbon ratio, mg N/mg C.

a_{NO_3C} = oxygen to carbon ratio for nitrate uptake, mg O_2/mg C.

a_{OC} = the oxygen to carbon ratio, mg O_2/mg C.

a_{ON} = oxygen to nitrogen ratio, mg O_2/mg N.

a_{PC} = phosphorus to carbon ratio, mg P/mg C.

bl = benthic layer, unitless.

BOD_{U5} = ratio of the ultimate to 5-day carbonaceous biochemical oxygen demand, unitless.

$CBOD_5$ = the internally computed 5-day CBOD, mg/L.

C_{ij} = constituent concentration advected between i and j, mg/L.

CJ = concentration of the water quality constituent in segment j, mg/L.

Cl = chlorides concentration, mg/L.

C_{pi}, C_{pj} = the particulate material concentrations in the benthic layer and water column respectively, mg/L.

C'_{PIP} = concentration of phosphorus sorbed to suspended solids, mgP/Kg SS.

C_{wi}, C_{wj} = the dissolved concentrations in the benthic interstitial waters and overlying water column respectively, mg/L.

DIP, DIN = available nutrients for growth, dissolved inorganic phosphorus (orthophosphate) and dissolved inorganic nitrogen (ammonia plus nitrate), mg/L.

DIP' = the new dissolved inorganic phosphorus resulting from the previous integration step, mg/L.

DO_{sat} = dissolved oxygen saturation, mg O_2/l.

D_{1j} = death rate, day^{-1}.

e = the natural logarithm = 2.71828, unitless.

E = the diffusive exchange rate between dissolved concentrations in the interstitial water and the overlying water column, ft^2/day.

E_{DIF} = diffusive exchange coefficient, cm^2/day.

Eij = dispersion coefficient between segments i and j, mi^2/day.

f = fraction of daylight, unitless.

f_{DIP} = the dissolved inorganic phosphorus pool, unitless.

f_{DOP} = the dissolved organic phosphorus pool, unitless.

f_{NH_3} = the ammonia nitrogen pool, unitless.

f_{ON} = the organic nitrogen pool, unitless.

f_p = the fraction of the total inorganic phosphorus assigned to the sorbed or particulate phase, unitless.

f_{POP} = the particulate organic phosphorus pool, unitless.

f_{pwc} = fraction particulate inorganic phosphorus, unitless.

G(I) = the light attenuation factor given by $G(I) = g(I,f,H,k_e)$, unitless.

G(N) = the nutrient limitation factor given by $G(N) = g(DIP,DIN)$, unitless.

G_{1j} = specific phytoplankton growth rate, day^{-1}.

G_{1max} = maximum Specific Growth Rate @ 20°C, day^{-1}.

H (or d in Figures) = the total water column depth, ft.

h = benthic layer depth, ft.

H_j = depth of the jth segment, ft.

I = incident solar radiation, ly/day.

I_a = the average daily solar radiation, ly/day.

I_o = the incident light intensity at the surface, ly/day.

$I_o(t)$ = instantaneous surfae solar radiation, ly/day.

k_a = reaeration rate @ 20°C, day^{-1}.

K_{aj} = reaeration rate coefficient at 20°C, day^{-1}.

$K_{aj}(T)$ = reaeration rate coefficient at ambient segment temperature, day^{-1}.

K_{BOD} = half saturation constant for oxygen limitation, mg O_2/L.

K_c = phytoplankton self-light attenuation; the extinction coefficient per unit of chlorophyll, m^2/mg chlorophyll-a.

k_d = deoxygenation rate @ 20°C, day^{-1}.

k_{DS} = organic carbon (as CBOD) decomposition rate, day^{-1}.

K_e = extinction or light attenuation coefficient, ft^{-1}.

K_e = the total extinction coefficient, computed from the sum of the non-algal light attenuation, K_e', and the self-shading attenuation due to ambient phytoplankton population, ft^{-1}.

K_{mN} = half saturation constant for nitrogen, µg N/1.

K_{mP} = half saturation constant for phosphorus, µg P/1.

K_{mPc} = half saturation constant for phytoplankton limitation, mg C/ℓ.

K_{nit} = half saturation constant for oxygen limitation, mg O_2/ℓ.

K_{NO_3} = Michaelis constant for denitrification, mg O_2/ℓ.

k_{OND} = organic nitrogen decomposition rate, day^{-1}.

k_p, k_w = first order reaction rates associated with the particulate and dissolved phases respectively, day^{-1}.

K_{PIP} = partition coefficient for particulate phosphorus, mgP/Kg SS.

k_{PZD} = anaerobic algal decomposition rate, day^{-1}.

k_{s1j} = the effective algal settling or loss rate, day^{-1}.

k_{1D} = a non-predatory death rate, representing the effect of parasitization, day^{-1}.

k_{1R} = algal endogenous respiration, day^{-1}.

$k_{1R}(T)$ = the algal respiration rate at 20°C, the temperature at which the field samples were incubated, day^{-1}.

$k_{1R}(20°)$ = the endogenous respiration rate at 20°C, day^{-1}.

k_{58} = dissolved organic phosphorus mineralization at 20°C, day^{-1}.

k_{68} = particulate organic phosphorus mineralization rate at 20°C, day^{-1}.

k_{140} = denitrification rate @ 20°C, day^{-1}.

k_{1013} = organic nitrogen mineralization rate @ 20°C, day^{-1}.

k_{1314} = nitrification rate @ 20°C, day^{-1}.

ℓ_{ij} = characteristic mixing length between segments i and j, ft.

P_c = the phytoplankton biomass in carbon units, mg/L.

PIP' = the sorbed inorganic phosphorus resulting from the previous integration step, mg/L.

P_j = phytoplankton population, cells/ℓ .

Q_{ij} = advective flow between segments i and j, defined as positive when leaving segment j, and negative when entering, ft^3/hr.

R_{ij} = dispersive flow between segments i and j, ft^3/hr.

S = concentration of suspended solids, Kg/L.

S_{kj} = kinetic transformations within segment j, mg/L/day.

S_{1j} = reaction term, cells/ℓ.day.

t = time, hr.

T = ambient water temperature, °C.

TIP = the total inorganic phosphorus, mg/L.

v_s = the net settling velocity of particulates across the water column-benthic interface, ft/day.

v_{sd} = the sedimentation velocity induced by sedimentation, ft/day.

v_{s1} = the net settling velocity of phytoplankton from the water column to the sediment, ft/day.

V_{tj} = average water velocity in segment j, ft/sec.

W = time-varying windspeed at 10 cm above surface, m/sec.

W_{Bj} = boundary loads into segment j, g/day.

wc = water column, unitless.

W_{Lj} = point and diffuse loads into segment j, g/day.

α_{NH_3} = preference for ammonia uptake term, unitless.

θ = the ratio of carbon to chlorophyll in the phytoplankton, (mg carbon/mg chlorophyll-a).

θ_a = temperature coefficient, unitless.

θ_d = temperature coefficient, unitlss.

θ_{DS} = temperature coefficient, unitless.

θ_{OND} = temperature coefficient, unitless.

θ_{PZD} = temperature coefficient, unitless.

θ_1 = temperature coefficient, unitless.

θ_{1R} = temperature coefficient, unitless.

θ_{58} = temperature coefficient, unitless.

θ_{68} = temperature coefficient, unitless.

θ_{140} = temperature coefficient, unitless.

θ_{1013} = temperature coefficient, unitless.

θ_{1314} = temperature coefficient, unitless.

ϕ_{max} = maximum photosynthetic quantum yield, $\frac{\text{mg C}}{\text{mole photon}}$.

ν = numerical weighting factor (0-0.5), unitless.

APPENDIX D

Symbols for Section 1.5

A = pre-exponential, or "frequency factor", unitless.

A_{ij} = benthic surface area, L^2.

A_{ij} = cross-sectional area between segments i and j, L^2.

A_s = surface area of water segment, L^2.

B_j = concentration of biomass in segment j, kg-biomass/L.

B'_j = concentration of biomass in water in segment j.
$B'_j = B_j/n_j$, kgb/L_w.

bl = benthic layer, unitless.

C = chemical concentration, ML^{-3}.

c = subscript for chemical, unitless.

C_{bj} = concentration of biosorbed chemical in segment j, mgc/L.

C'_{bj} = concentration of biosorbed chemical in biota in segment j.
$C'_{bj} = C_{bj}/B_j$, mgc/kgb.

C_G = cloud cover, tenths of sky (1-10).

C_{ij} = constituent concentration advected between i and j, ML^{-3}.

C_j = concentration of total chemical in segment j, mgc/L.

C_{PO4} = dissolved inorganic phosphorus concentration, µg/L.

C'_s = sorbed chemical concentration, $MM^{-1}{}_{sediment}$.

C_{sj} = concentration of sorbed chemical in segment j, mgc/L.

C'_{sj} = concentration of sorbed chemical on sediment in
segment j. $C'_{sj} = C_{sj}/S_j$, mgc/kgs.

C'_w = dissolved chemical concentratin, $ML^{-3}{}_{water}$.

C_{wj} = concentration of dissolved chemical in segment j, mgc/L.

C'_{wj} = concentration of dissolved chemical in water in segment j. $C'_{wj} = C_{wj}/n_j$, mgc/L_w.

D = average depth of the water segment, m.

d = optical path, cm/cm.

d_p = particle diameter, mm.

E_a = Arrhenius activation energy, kcal/mole.

E_{DIF} = diffusive exchange coefficient, cm^2/sec.

E_{ij} = dispersion coefficient between segments i and j, such as cm^2/sec, m^2/hr, or mi^2/day.

$[E]_k$ = the intensity of environmental property affecting process "k", such as light intensity or bacterial population.

f_B = fraction of population actively degrading organic compound, unitless.

f_{ocB} = organic carbon fraction of biomass, unitless.

f_{ocs} = organic carbon fraction of sediment, unitless.

f_{pbl} = fraction particulate in the sediment layer, unitless.

f_T = the spatially variable proportionality constant between pore water dispersion and sediment mixing (0-1), unitless.

g = acceleration of gravity = 981 cm/sec^2.

H = Henry's Law constant, atm-m^3/mole.

h = benthic layer depth, ft.

i = benthic segment, unitless.

I_{Gk} = average light intensity of wavelength k, E/cm^2-sec.

I_m = average light intensity within water segment, E/cm^2-sec.

I_o = surface light intensity, E/cm^2-sec.

j = water segment, unitless.

k_a, k_b = specific acid and base catalyzed rate constants, respectively, $molar^{-1} \cdot hr^{-1}$.

k_{ai} = specific sunlight absorption rate for phase i, E/mole-hr or (E/L)/(mole/L)/hr.

K_{Bs} = net biodegradation rate constant in benthic segment, hr^{-1}.

K_{Bw} = net biodegradation rate constant in water segment, hr^{-1}.

k_d = desorption rate constant, hr^{-1}.

K_e = spatially variable light extinction coefficient, m^{-1}.

K_H = net hydrolysis rate constant, hr^{-1}.

k^i_{Bs} = second order biodegradation rate constant for phase i in benthic segments, ml/cell-hr.

k^i_{Bw} = second order biodegradation rate constant for phase i in water segments, ml/cell-hr.

k^i_o = second order oxidation rate constant for chemical phase i, L/mole-hr.

k_k = secnd-order rate constant for process k.

k_n = neutral rate constant, hr^{-1}.

K_o = net oxidation rate constant, hr^{-1}.

K_{oc} = organic carbon partition coefficient, (L_w/kg_{OC}).

K_{OPD} = organic phosphorus decomposition rate, day^{-1}.

K_{o2} = temperature corrected reaeration velocity, m/hr.

K_{pB} = partition coefficient of chemical on biomass, L_w/kgb.

K_{pG} = first order photolysis rate coefficient at reference light intensity, hr^{-1}.

K_{ps} = partition coefficient of chemical on sediment in segment j, L_w/kgs.

K_v = net volatilization rate constant, hr^{-1}.

k_v = conductivity of the chemical through the water segment, m/hr.

K_{20} = reaeration velocity at 20°C, m/hr.

[L] = fraction of reference light I_G in segment (I_m/I_G), unitless.

L_c = latitude correction factor, calculated internally, unitless.

ℓ_{ij} = characteristic mixing length between segments i and j, ft.

MW = molecular weight of the compound, g/mole.

n_{ij} = average porosity o segments i and j, $L^3_{water}L^{-3}$.

n_j = porosity or volume water per volume segment j, L_w/L.

P = sediment wet weight to dry weight ratio, M (sediment + water), M^{-1} (sediment).

P_{bac} = bacterial population density in segment, cell/ml.

P_i = transformation product for process k, unitless.

Q_{ij} = advective flow between segments i and j, defined as positive when leaving segment j, and negative when entering, L^3T^{-1}.

Q_{pj} = pore water flow generated by sediment compaction, L^3T^{-1}.

Q_{ps} = pore water flow from compaction, L^3T^{-1}.

Q_{Ts} = "Q-10" temperature correction factor for biodegradation in benthic segments, unitless.

Q_{Tw} = "Q-10" temperature correction factor for biodegradation in water, unitless.

R = ideal gas constant = 8.206 x 10^{-5} m^3-atm/mol°K.

R_{Bij} = pore water diffusive exchange flow, L^3T^{-1}.

R_G = gas phase resistance, hr/m.

R_{ij} = dispersive flow between segments i and j, L^3T^{-1}.

R_L = liquid phase resistance, hr/m.

$[RO_2]$ = molar concentration of oxidant, moles/L.

S = sediment concentration, ML^{-3}.

s = subscript for sediment, unitless.

S'_i = sediment concentration per unit pore water, ML_w^{-3}.

S_j = concentration of sediment in segment j, kgs/L.

s_j = concentration of sediment in segment j, mgs/L.

S'_j = concentration of sediment in water in segment j, $S'_j = S_j/n_j$, kgs/L_w.

S_{kj} = kinetic transformations within segment j, $ML^{-3}T^{-1}$.

T = ambient temperature in segment, °C.

t = time, T.

T_{ij} = sediment turnover rate, MT^{-1}.

t_{ij} = average tortuosity of benthic segments i and j, $L_{water}\ L^{-1}$.

t_{ij} = average tortuosity of segments i and j, $L_{water}L^{-1}$.

T_k = water temperature, °K.

V = volume of the water segment, m^3.

V = average segment velocity, ft/sec.

V_j = volume of segment j, L^3.

V_s = Stokes velocity for particle with diameter d_p and density ρ_p, m/day.

W = wind speed at 10 cm above surface, m/sec.

W = time-varying windspeed at 10 cm above surface, m/sec.

WAT = water vapor exchange velocity, m/hr.

W_{Bj} = boundary loads into segment j, MT^{-1}.

wc = water column subscript, unitless.

w_D = deposition velocity, LT^{-1}.

W_{Lj} = point and diffuse loads into segment j, MT^{-1}.

w_R = scour velocity, LT^{-1}.

w_{sedij} = sediment velocity in bed, positive leaving j, negative entering j, LT^{-1}.

w_{sij} = settling velocity in water, positive leaving j, negative entering j, LT^{-1}.

W_z = wind speed at height z, m/sec.

Y_k = yield coefficient for process k, unitless.

z = measurement height, m.

α_i = fraction of chemical in phase i, unitless.

α_D = probability of deposition upon contact with the bed, unitless.

α_1 = dissolved fraction of the chemical, unitless.

$\alpha_1, \alpha_2, \alpha_3$ = fraction of chemical in each phase, unitless.

ϵ_k = molar absorptivity of wavelength k, m 10-L/cm . mole.

θ_{OPD} = temperature coefficient, unitless.

μ = absolute viscosity of water = 0.01 poise (g/cm^2-sec) at 20°C.

ν = numerical weighting factor, 0-0.5, unitless.

ρ_B = bulk density, kg (sediment and water)/L.

ρ_s = sediment density ≈ 2.7 kg/L_s.

ρ_w = water density ≈ 1 kg (water)/L_w.

ϕ_{pi} = reaction yield fraction for chemical in phase i, unitless.

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